Chapter 4

EMISSION SUBSYSTEM

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ABSTRACT

Chapter 4 provides a description of the Models-3 Emission Processing and Projection System (MEPPS) structure, scientific approach and the assumptions used in modeling and processing emission data in the Models-3 framework. The description includes emission data entry through the Inventory Data Analyzer (IDA) import and quality control checks; and the data flow and quality control used in loading emission inventory and meteorology data in the MEPPS Input Processor. The description of the main Emission Processor addresses the basis of spatial and temporal allocation procedures. The scientific models and assumptions used in modeling hourly mobile source and biogenic emissions are explained (Biogenic Emission Inventory System 2 and Mobile 5a, respectively). The rationale and assumptions are described which are used in the allocation and grouping of individual chemical species into "lumped species" in preparation for the lumped species chemical transformation mechanisms contained in the Community Multiscale Air Quality (CMAQ) model. The chapter also describes the procedures used by the Models-3 Emission Projection Processor to estimate emission data for use in modeling future air quality scenarios. Finally, the quality control report and output file options contained in the Output Processor are described.

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4.0 EMISSION SUBSYSTEM

The rationale for the Models-3 air quality emission processor is rooted in the need to estimate, organize, and process emission inventory data for regulatory and scientific analysis and modeling. Historically, air quality emission processing methods have been developed in an ad hoc manner, with each procedure specifically tuned to meet the need at hand, reflecting the various data information sources and estimation methodologies, as well as the uses of the data. The Models-3 air quality emission processor consolidates and simplifies the estimation, data handling, and linkage of the resulting data to air quality models. This section describes the purpose, origins, and scientific bases of the Models-3 Emission Projection and Processing System (MEPPS). Material is presented in the general sequence of emission processing. System requirements, system design ,and detailed user information for emission data processing are not addressed in this Volume. These items are described in Volume 7, Volume 8, and Volume 9B, respectively of the Models-3 documentation set. For example, processor names, environment variables, and flow diagrams are given in Chapter 6 of the *Models-3 Volume 9B: User Manual*.

4.1 Emission Inventory Processors

In the Models-3 framework, MEPPS imports, quality controls, and processes emission inventory data for either direct regulatory analysis or input to a chemical transport model. The MEPPS also models hourly biogenic emissions and mobile source emissions. The MEPPS is non-conforming within the framework because it is not an object-oriented component, and because it does not use the NetCDF Input/Output Applications Program Interface (I/O API) format internally. Processing is accomplished using a combination of FORTRAN, SAS®, and ARC/INFO® programs. The emission processor results are translated into the NetCDF I/O API format by the MEPPS Output Processor.

4.1.1 Discussion

The MEPPS builds on lessons from and functionalities of previous software developed for processing emission inventories. The capabilities and design decisions in MEPPS are placed in the context of emission inventory developments.

4.1.1.1 The Role of Emission Inventory Processing for Chemical Transport Modeling

Historically, there have been many air quality emission data bases which were compiled and used for the purposes of regulatory or scientific assessment of emissions, including spatial and temporal patterns and trends. As air quality chemical transport models (CTMs) were developed, each had its own specific format for input data, based either on the data structure used in the model and/or the format of the available data. Initially, CTMs were relatively simple and applied to one or a few point sources, such as emissions from an industrial stack. As CTMs for urban and regional scales - such as the Urban Airshed Model (Morris et al.,1992) - became more sophisticated, the level of detail needed for input emission data became increasingly more

comprehensive and detailed. It became necessary to include as complete an inventory as possible for the area of interest, including emissions from all diffuse as well as point sources at as great a degree of spatial and temporal resolution as possible. As the spatial and temporal resolution of the models has increased, so has the demand for detailed emission input data. Because of resource limitations on data gathering, the emission inventory information needed often substantially exceed the reported or observed emission data available. The result is development of a wide range of emission estimation and modeling techniques.

Emission inventory data are available from various sources, often state and local air pollution control agencies. The data are commonly compiled into annual emission inventories for specific areas to be analyzed and/or modeled. The spatial extent of an emission inventory may vary from plant-specific emission data to data for an entire country or more. Recent regional examples include the National Acid Precipitation Assessment Program 1985 National inventory (Saeger et al.,1989), the 1990 EPA Interim National Emission Inventory (U.S. EPA, 1993; U.S. EPA, 1994), and the 1990 Ozone Transport Assessment Group inventory (Ozone Transport Assessment Group, 1997). Most emission inventories are organized into four traditional general groups of emission types:

- Point sources, which are emission sources attributable to discrete emission points, usually a stack. The data include pollutant, source category code, stack parameters (height, diameter, exit velocity, temperature, flow rate), emissions, location coordinates, fuel, etc.

- Area sources, which are emission sources attributable to diffuse sources or areas, such as agricultural fields, large open mining operations, forests, or a combination of many point sources which are too small and numerous to account for individually (e.g., residences). Area source inventories are typically by county and include pollutant, source category code, emissions, location, coordinates, etc.

- Biogenic sources, which are often natural emissions from vegetation, soils, and lightning. Biogenic emissions are dependent on temperature, solar radiation, and land cover type. They are usually modeled hourly for specific days and locations.

- Mobile sources, which are emissions from vehicular traffic on roadways, aircraft, trains, shipping, and off-road mobile equipment. Mobile source emissions are dependent on the ambient temperature, road type, vehicle type and age, miles traveled, etc. These emissions are generally modeled for specific day and meteorology scenarios either by county or road segment (link-node data).

The techniques used to estimate emissions in compiling an emission inventory are based on extrapolation of limited direct measurements for point sources, and application of limited measurements or estimates to spatial surrogate data for area sources. Emissions which are dependent on environmental conditions (e.g., biogenic and mobile source emissions) are modeled to generate either portions of emission inventories or hourly data for direct use in air quality

modeling. The procedures used to process emission inventory data and to model and process mobile and biogenic source emission data are described in more detail in the following sections.

Point source and area source emission inventory data are usually included in annual emission inventories. Annual mobile and biogenic emissions are included if the inventory was intended for assessing annual totals or trends of emissions. If the inventory was prepared for modeling, only the annual "Vehicle Miles Traveled" by county or road segment and vegetation land cover may be provided. In order to accomplish episodic air quality modeling, it is necessary to model the hourly mobile and biogenic emissions for the episode-specific meteorological conditions.

The typical procedures used to prepare annual emission inventories for use in a CTM require temporal, spatial, and pollutant species allocation of the data. This is accomplished in a sequential manner. For regional modeling, initial "raw" emission inventory data files are very large, often several megabytes in size. The data files are subjected to a variety of data quality checks, depending upon the methodological sophistication and computing and time resources available. Typically, visual inspections of mapped locations, value range checks, cross-checks of sums, and routine computer checks for blank fields and valid data types are performed.

In order to reduce the size of emission data files, the data are often speciated first, depending upon the pollutants involved, then temporally allocated to hourly data, and then spatially allocated or "gridded" to a spatial domain with gridded cells of the resolution required by the CTM. At each step some of the detailed information, such as source category code and geographic coordinates, are dropped to reduce the file size. Hourly mobile source and biogenic emission data are modeled using the appropriate hourly meteorological data, and merged with point and area source data prior to speciation.

It is necessary to rerun the processing sequence in the event of an error, or for each new meteorological or day-specific scenario. Projections to future years require application of source-category-specific economic growth factors to a base year inventory to produce a projected annual inventory. The projected inventory is then processed through the entire emission processing sequence. Preparation of detailed regional emission inventory data for regional modeling using this traditional approach may take weeks or month.

4.1.1.2 Function and Place of the Emission Processor in the Models-3 Framework

The Models-3 framework is designed to contain conforming object-oriented modules that pass data in the NetCDF I/O API format, although non-conforming modules are accommodated at the cost of reduced functionality. The emission processing system is intended to ultimately be conforming. The initial version of MEPPS was derived from existing software and consequently is not a conforming object-oriented program in Models-3. However, it is integrated into the Models-3 framework and does take instructions and information from the system and provides emission data output in NetCDF IO/API format. Figure 4-1 provides a functional view of the Models-3 system. Processing of emission data is often a part of iterative air quality strategy

building, directly or indirectly, though the effect of emissions on air quality modeling results. Figure 4-2 is a simplified illustration of the location of MEPPS and other non-conforming components within the Models-3 framework. The main aspects of a study (including the principal emission processing options) are graphically defined in the high-level Models-3 Study Planner, and the resulting information is automatically passed to MEPPS as well as other portions of the system. Specifically, a study name is defined by the user by copying, modifying, and renaming an existing "template" emission study. For example, a tutorial emission study could be used as a template to define a new study. The new study is associated with input data sources, MEPPS processing and modeling modules and their primary options by annotating links and nodes in the specified emission study and plans. The pollutants of interest, the geographic domain, map projection, grid spatial resolution, chemical speciation mechanism, temporal resolution, and dates of interest (referred to as the "case") are defined in the Models-3 Science Manager and passed to the rest of the system including MEPPS. This approach allows the user to make primary specifications once, rather than separately to each of the system components and thus ensures consistency. Study Planner and Science Manager also aid in using the system to run multiple emission, projected emission, and emission control scenarios without frequent respecification of parameters. From a functional view, MEPPS generates emission data that reflect user-defined studies and cases, whether for regulatory analysis of emission data and/or for input to CTM runs and comparison with CTM results.

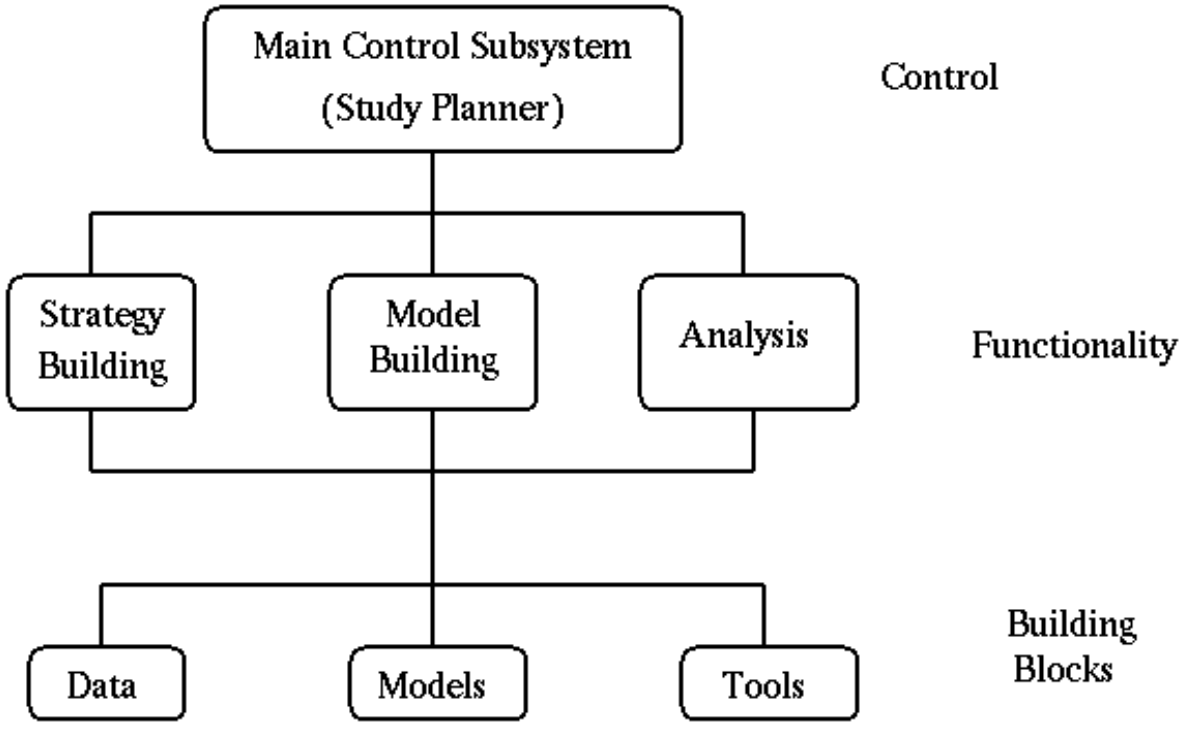


Figure 4-1 Functional View of the Models-3 System

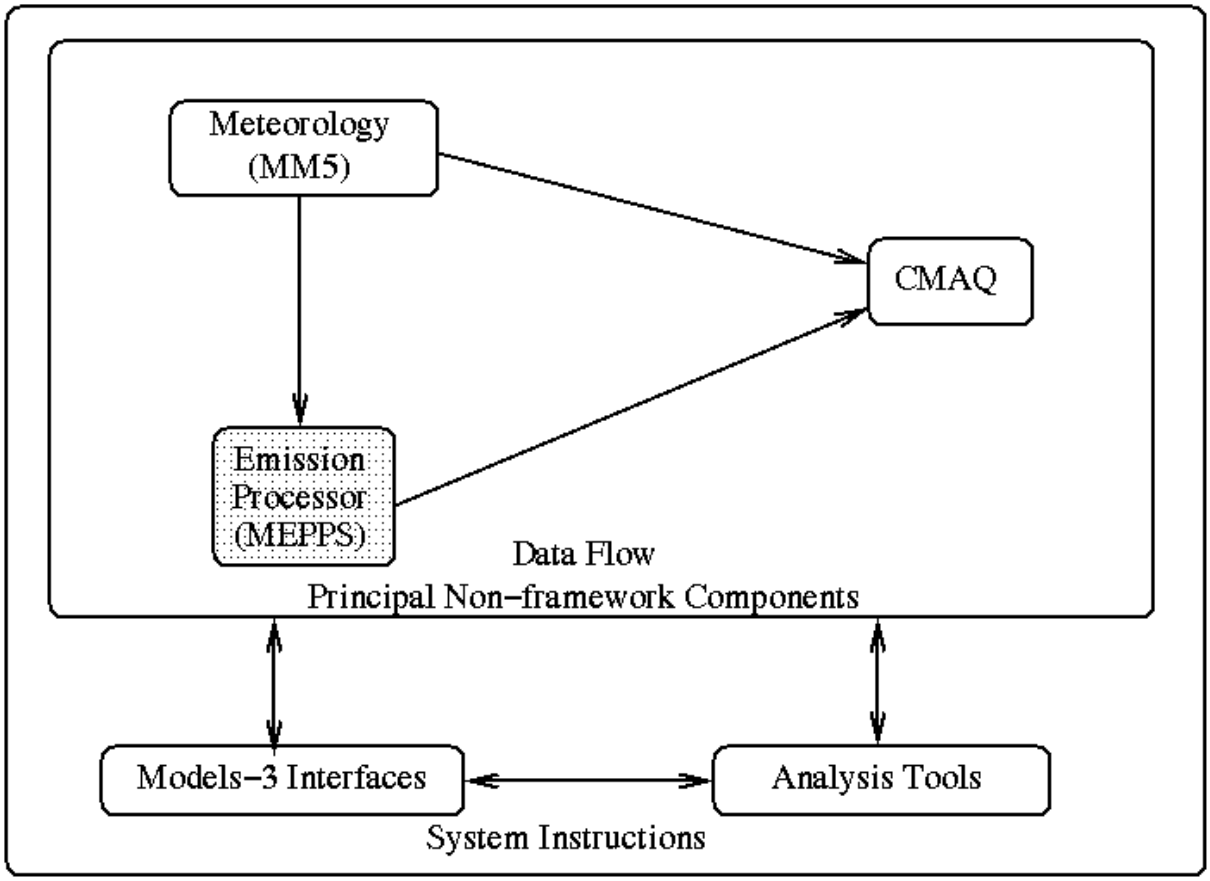
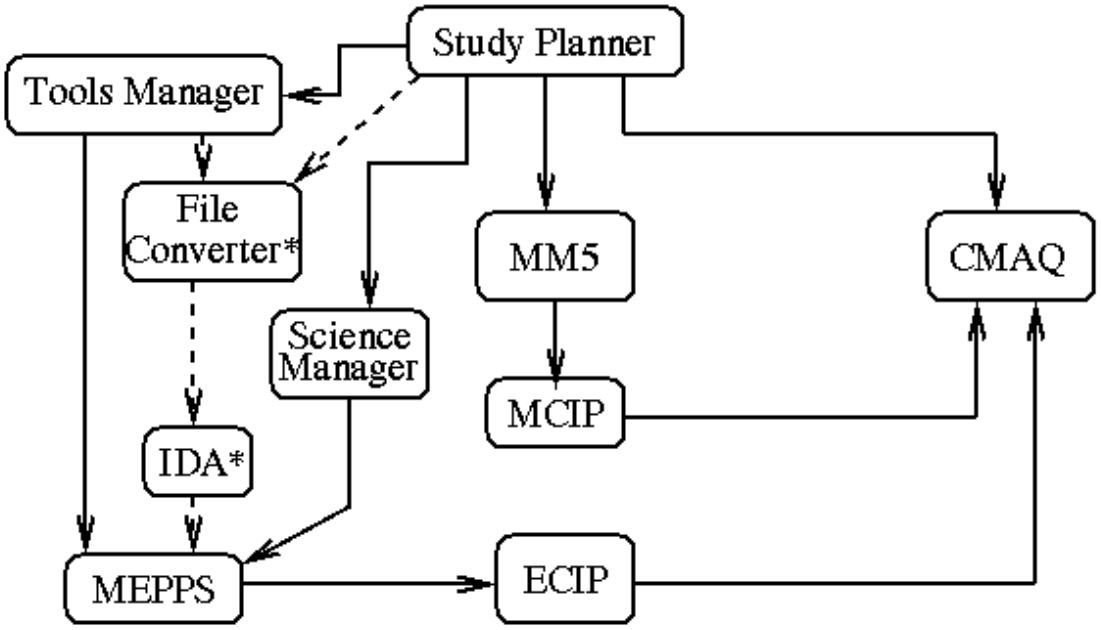


Figure 4-2 The location of MEPPS within the Models-3 Framework

The emission processing function of MEPPS requires that it be linked to the Models-3 framework, and to other processing, modeling, and analysis tools through the framework. MEPPS outputs data in the NetCDF I/O API format in order to link MEPPS to the Models-3 framework and other processing, modeling, and analysis modules. Figure 4-3 illustrates that information (grid, chemical mechanism, and case) user-specified in Models-3 Science Manager for a study is passed to other modules, including MEPPS. However, it is necessary to access the Parameter Window of MEPPS through the Tools Manager, to specific study name, grid, source (data source name), and case, and then return to the Study Planner to run the emission study. Direct access to MEPPS is through the Tools Manager and the emission projection and control functions are in Strategy Manager. New emission inventory data are imported and quality controlled through the Models-3 File Converter and its subsidiary Inventory Data Analyzer (IDA). The data are then imported directly into MEPPS through its internal Input Processor (INPRO). Meteorological information needed to estimate biogenic and mobile source emissions are provided to MEPPS from a meteorological model or dataset in the Models-3 system through

the Meteorology-Chemistry Interface Processor (MCIP). For regional-scale modeling, the current default meteorological model is Mesoscale Model 5 (MM5). The MEPPS processes emission data into speciated, spatially and temporally allocated hourly emission data for use in a Models-3 conforming CTM. The data are output as NetCDF I/O API files to the Emission-Chemistry Interface Processor (ECIP) which adjusts the format to that needed by the CTM. Emission data for large elevated point sources (large stack emissions) are also provided as I/O API files to the Plume Dynamics Module, and the plume rise algorithm.



Where: MM5 is Mesoscale Model 5
CMAQ is Community Multiscale Air Quality Model
MEPPS is Models-3 Emission Processing and Projection System
MCIP is Meteorology-Chemistry Interface Processor
ECIP is Emissions-Chemistry Interface Processor
*IDA is Inventory Data Analyzer
*File Converter is generic to the Models-3 system
*IDA and File Converter are optional (used for new data)

Figure 4-3 Relationship of Principal Models-3 Framework Components

4.1.1.3 Rationale for the Basis of the Initial Version of MEPPS

In order to assure that an acceptable and functional emission inventory processor would be present in the initial release of Models-3 given time and resources available, it was decided that the emission processing module for the initial version would be based on software and methodologies available as of 1994. More advanced approaches being researched and developed then and now will be incorporated as soon as possible. The decision factors used in selecting

from existing emission processors were availability, cost, features (capabilities), hardware and software requirements, and operating characteristics. Table 4-1 lists the emission processing systems considered with respect to the principal evaluation factors.

Based on the evaluation, the Geocoded Emission Modeling and Projection System (GEMAP; Wilkinson et al.,1994), now known as the Emission Modeling System-95 (EMS-95), was selected as the basis of the initial emission processing system, although it is non-conforming (not in I/O API Net CDF) in the Models-3 system. The GEMAP was selected because it was readily available in the public domain; it was state-of-the-art at the time; there was no licensing cost (exclusive of GEMAP's internal use of SAS® and Arc/Info®); its code was modular and flexible; and it contained a geographic information system to perform spatial allocation of emission inventory data.

Other systems considered included the Emission Processing System (EPS), The Flexible Regional Emission Data System (FREDS), and the Sparse Matrix Operator Kernel Emission System (SMOKE). The EPS is used to process emission inventory data for the Urban Airshed Model (UAM; U.S. EPA, 1992). A recent adaptation of EPS by Environment Canada for regional use is called the Canadian Emission Processing System Version 1 (CEPS1.0) (Moran et al., 1998). Like GEMAP, EPS would be non-conforming code in the Models-3 framework, and would require design and development of interfaces with the Models-3 system and the addition of many features. However, EPS does not include flexible GIS-based gridding capability of GEMAP and was originally designed for urban scale air quality modeling as opposed to the multiscale (local to regional and national) air quality modeling capabilities of Models-3.

The FREDS has been used for regional air quality modeling during the past ten years in conjunction with the Regional Oxidant Model and Regional Acid Deposition Model (Modica et al., 1989). The FREDS code is run on a main-frame computer, and is "hard-wired" and difficult to change for different scenarios or grids. Consequently it lacks the modularity and flexibility needed to operate in the Model-3 framework.

Design and prototyping of SMOKE was just beginning when the design of the initial version of Models-3 was determined (Coats, 1995). The SMOKE, which is now being used in conjunction with UAM, could be modified to be fully compliant with the object-oriented Models-3 system. Additional analysis and quality control tools are being designed for SMOKE, and initial work has begun to adapt it to the Models-3 framework.

Table 4-1. Emission Processor Selection Factors for the Initial Public Release of Models-3

Factors	Emission Processing System (EPS)	Flexible Regional Emission Modeling System (FREDS)	Geocoded Emission Modeling and Projection System	Sparse Matrix Operator Kernel Emission (SMOKE) system
Acquisition Cost of Source Code[1]	None	None	None	N/A
Availability	Public domain	Public domain	Public domain	N/A
Degree of Development	Completed and in use	Completed and in use	Initial version being tested	Design and prototype beginning
Relative Flexibility for Modification to Models-3	Changes required recoding of modules to allow revised interfaces and external control - spatial allocation would be added	Changes required substantial recoding - many patches - relatively inflexible -spatial allocation would be added	Changes required recoding of modules to allow revised interfaces and external control - spatial allocation already present	N/A
Hardware Requirements	Work station with UNIX operating system	IBM Mainframe system	Work station with UNIX operation system	Unix-based machines, specifics not established
History (Operating Experience)	Established system used by EPA, state, and local agencies	Established system used by U.S. EPA in regional modeling programs	New system, used only with test data in California	N/A
Software Requirements	FORTRAN and SAS®	FORTRAN and SAS®	SAS® and ARC/INFO® licenses.	Unix-based, specifics not well established
Spatial Allocation Capability	Spatial allocation grids must be manually coded for each allocation scenario.	Spatial allocation grids must be manually coded for each allocation scenario.	ARC/INFO® allows flexible user-defined grid domains, spatial resolution and data overlays	Unknown

Since its selection, GEMAP/EMS-95 has been substantially modified and incorporated into MEPPS. Because of the changes, the GEMAP portion of MEPPS has been renamed the Emission Processor (EMPRO) module. Revisions were made to allow the software to be more generic and efficient in its operation, and new features were added. In general, new capabilities were written in FORTRAN and placed in modules outside of GEMAP. This was done to minimize rewriting of code in future when the GEMAP-based portion of the system is replaced.

MEPPS must include several basic functions. There are also many enhancements, detailed descriptions for which may be found in Volumes 7, 8, and 9 (System Requirements, System Design, and User Manual, respectively) of the Models-3 documentation set. The experience and design suggestions of personnel familiar with processing large emission inventories were used as important guidance in deciding which features to include in MEPPS. The design and implementation of MEPPS emphasized ease of use and efficiency within the overall design of the Models-3 system. The following paragraphs present a brief description of the principal functions included in MEPPS.

- Annual point and area source emission data from inventories are subset to the spatial domain of interest, spatially allocated to a grid, and temporally allocated. Area source emissions are spatially allocated using surrogate spatial coverages.

- Spatial allocation of each general type of air quality data (point, etc.) to grid cells is done by the GIS using a grid defined by the Science Manager module of Models-3.

- Modeled estimates of mobile source emissions are prepared on an hourly basis for periods of interest, usually several days. These estimates account for meteorological conditions using data from a meteorology model (such as MM5) that has been passed through the Models-3 meteorology-chemistry interface processor (MCIP). Hourly, grid-cell specific emission factors for different vehicle and roadway classifications are prepared with MM5 using vehicle miles traveled (VMT) data from an emission inventory.

- Modeled hourly estimates of biogenic source emissions are prepared on an hourly basis for periods of interest, using the Biogenic Emission Inventory System Version 2 (BEIS-2) and meteorology data from MCIP and land use coverages (see Section 4.2.4.1).

- Temporal allocation of emission data to hourly data for the period of interest is accomplished using source-type specific defaults or user-selected temporal allocation profiles.

- Disaggregation of gridded, temporally-allocated emission data of groups of chemical species to specific species (chemical speciation) is completed according to the users choice of chemical speciation mechanism (currently Carbon Bond 4 (CB-4) and RADM 2.0).

- Projection of emission inventory data to future years from a base-year inventory (1990) and application of controls is performed by the Models-3 Emission Projection Processor (MEPRO). Projected emission inventories are used to iteratively evaluate different emission scenarios caused by economic or emission control changes. Projected emission inventories are each processed by MEPPS for air quality modeling in the same way as the original, or "base" inventory.

- Merging of spatially and temporally-allocated, speciated files for point, area, mobile, and biogenic emission data into one emission data output file, and translation into NetCDF I/O API format are performed for use in the Models-3 system, including the chemical-transport model. Summary and quality control reports on the output data are also produced.

- User-defined point-source emission data are extracted and prepared for use in vertically-layered (three-dimensional) emission files to be used with the plume dynamics module of the Models-3 system.

4.1.2 General MEPPS Structure

The MEPPS is normally used as an integral part of the Models-3 framework from high-level menu-driven screens and pick-lists.

MEPPS in the Models-3 Framework

A user may define a study using the Study Planner within Models-3. The Study Planner specifies the name and description of a study, and defines data sources, models, and the relationship between them using a graphical interface. If a study includes processing of emission data, the sequence of processing operations, source file addresses and many options for processing are defined by the Study Planner and passed to MEPPS annotated to the study name. Specifications for spatial allocation grids, and definition of specific temporal cases are defined in the Science Manager. Existing studies, grids, work space directories, speciation mechanisms, source directories, and computer hosts must be selected from the MEPPS parameter window located through the MEPPS icon in the Tools Manager prior to running under the Study Planner. The MEPPS may also be directly accessed through the Tools Manager and run interactively via its SAS® interface windows. During direct access interactive operation, some features may be run individually in the background using an “interactive” batch mode selection, or a series of processes may be run together as a concatenated batch run.

The MEPPS shares an import File Convertor with the rest of the Models-3 framework. The File Convertor will import any ASCII, SAS®, or NetCDF I/O API file of format known to the user. SAS® data sets are used within EMPRO. The data are imported, converted, and subjected to basic quality control checks, including missing or out-of-range values. The data are then put through the Inventory Data Analyzer (IDA) for quality control and analysis specific to emission files,

including inventories (in one of four EPA formats), temporal allocation factors, control factors, vehicle miles traveled, and continuous emission monitoring (CEM) data. The data then go to the MEPPS Input Processor (INPRO) for final quality control and loading into EMPRO.

The Internal Components of MEPPS

The emission processor (MEPPS) includes several basic components (Figure 4-4): an emission data Input Processor (INPRO), a main Emission Processor (EMPRO), an Output Processor (OUTPRO), and a Models-3 Emission Projection Processor (MEPRO). The File Converter and IDA are not intrinsic parts of MEPPS. They are used to import, quality control, and convert the formats and units of data files of known format to the formats that are used in the Models-3 system, including emission inventories and related emission data files. The INPRO imports emission inventory data from IDA and meteorology files from MCIP, and prepares them for use in EMPRO. The EMPRO spatially and temporally allocates point and area source emission data to hourly gridded data. It is also used to model biogenic and mobile-source emission data using meteorological data generated by MM5 and processed by MCIP, as well as spatially and temporally allocates the data. The EMPRO then allocates (groups) the chemical species from the gridded temporally allocated emission files according to the user's selection of a chemical speciation mechanism. The speciated files then go to OUTPRO where they are merged (a two-dimensional file). Quality control is performed and summary reports are prepared in accordance with the user's choices. The user also may divide point sources into categories to separate very large sources (major-elevated point sources or MEPSE) and large sources (major sources) into separate output files, which may be placed in a three-dimensional emission output files to be allocated to vertical layers for CMAQ. The user defines what is MEPSE or major using a combination of pollutant-specific emission values and/or stack parameters (see Section 4.2.6). Remaining point sources are merged into the two-dimensional emission output file along with area, mobile, and biogenic source emission data. Output files are in NetCDF I/O API format. The MEPRO module projects emission inventory data to future years while applying controls. The projected emission data can be read by EMPRO for further processing if modeling of a projected case is desired

4.2 The MEPPS Emission Processing System

Although MEPPS is a significant advance in emission inventory data processing, it is continually being improved. The following sections describe the scientific rationale for the 1998 (first public release) version of the system.

This section describes the basis for emission processing procedures in MEPPS. For models developed independently of the Models-3 framework and incorporated into MEPPS, documentation for those models is referenced. MEPPS was developed to meet emission processing needs specified in *Models-3 Volume 7: Design Requirements* of the Models-3 documentation set, as amended. The design requirements for emission inventory processing are based on the emission data input requirements of chemical transport models, and on the needs of

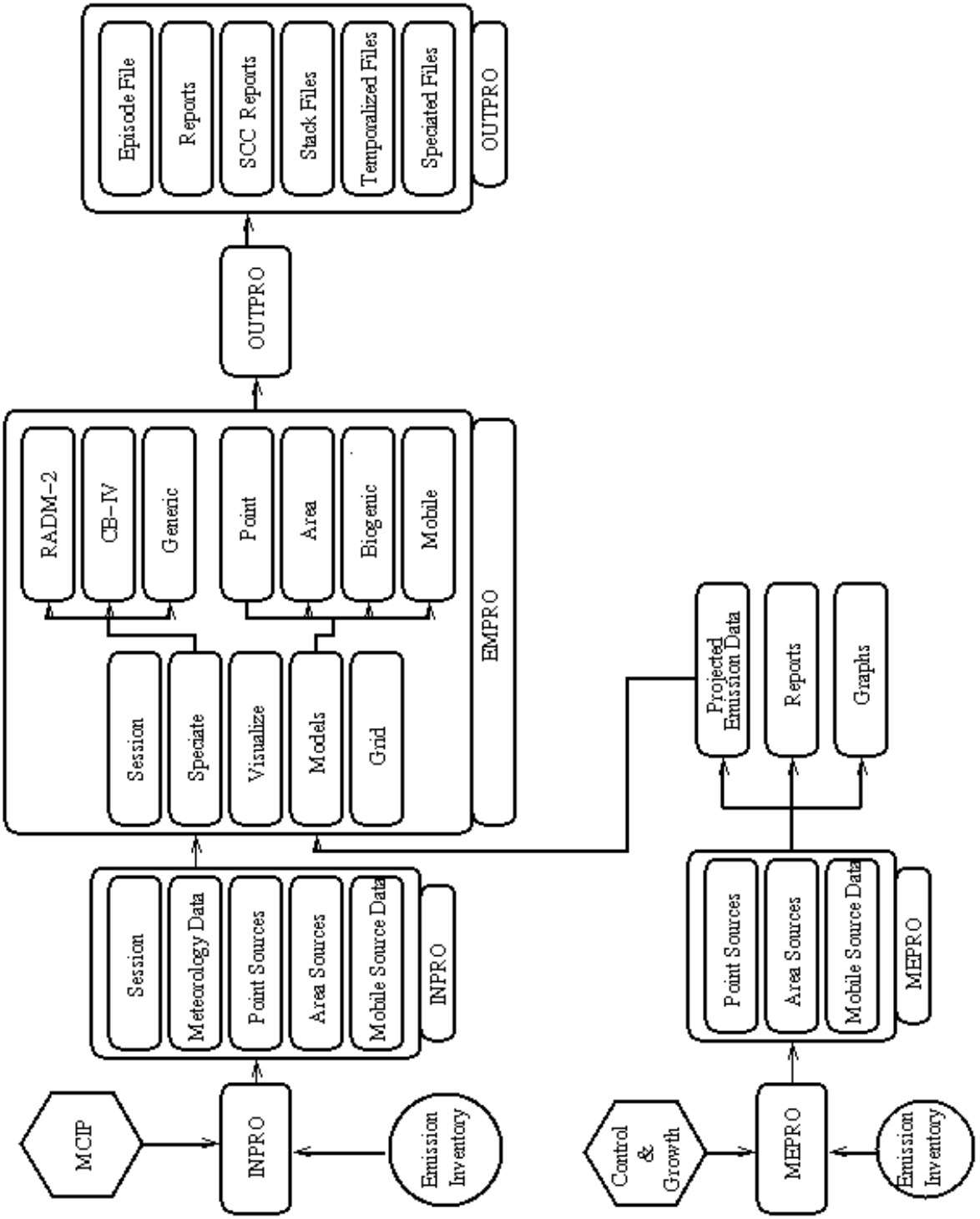


Figure 4-4 Functional Components of MEPPS

those who will use MEPPS to process emission data for both regulatory and scientific emission analysis as well as CMAQ data input. Two guiding principles were followed in the design and implementation of MEPPS. First, substantive changes to the existing GEMAP system were minimized because of a long-term goal to replace GEMAP with a more flexible, less costly (in terms of software licenses), and faster processor. Changes focused on improving the processing efficiency and correcting basic inadequacies of GEMAP. The second principle was to place new features and new emission processing developments outside of GEMAP to the extent possible, but within MEPPS. The resulting structure will make it easier to replace the GEMAP-based portion of MEPPS in the future.

MEPPS is usually run from the Models-3 Study Planner, although it can be run independently in interactive mode. Consequently, MEPPS is configured to run in a "batch" mode (from Study Planner for multi-day cases), and to accept Study Planner specifications for emission data processing and location of data sources. Some MEPPS processors that may be run when accessing MEPPS through the Tools Manager (such as file, grid, and case creation, deletion, or editing), will not function when MEPPS is accessed through the Study Planner. This provision avoids conflicts when these processes are specified from the Models-3 framework under Science Manager. The main components of MEPPS are each discussed in the following sections.

4.2.1 The Inventory Data Analyzer (IDA)

The IDA is an important enhancement to Models-3. It operates as an adjunct to the generic File Converter, which is described in Section 10.8 of the Models-3 User Manual (Volume 9b of the Models-3 documentation set). The File Converter is fully-compliant component of Models-3, applicable to the entire system, and provides file format and unit conversion for files imported into or exported from Models-3, including emission related files. The formats currently used in Models-3 and supported by the File Converter are NetCDF I/O API (gridded data), ASCII, and SAS®.

The IDA imports files from the File Converter and provides quality control and analysis tools specialized for reading, comparing, editing, and analyses of emission data . Quality control reports are generated including the results of the checks. Emission inventories that are in terms of annual, daily, or hourly emissions can be imported. The functionality of IDA is fully described in Section 6.2 of the User Manual. Specific quality control functions include the following:

- Range checks. Ranges accepted by IDA were taken from the range of values known to be correct in inventories currently in the system (1985, 1990, 1995). English units are used because most U. S. inventories are submitted with those units. Values outside of the validity ranges are considered incorrect. The validity ranges currently used in IDA for point-source stacks are:

Diameter	>0.5 and < 50 ft.
Diameter	< 0.2 * Height
Height	>1.0 and <1,250 ft.
Temperature	>50 and <2,000°F
Velocity	>1 and <1000 ft/sec
Flow rate	>1 and < 30,000,000 ft^3/sec and/or

Flow rate must not be more than 10 percent different from flow rate calculated from Velocity and Diameter.

- Sign checks. The system reports suspect signs based on the knowledge that particular parameters are always of a given sign (e.g., stack height are positive).

- Missing data checks. The system automatically fills missing data with Source Category Code-specific default data generated from the inventory being processed.

- Incorrect data checks. Data are corrected automatically when they can be computed based on specific mathematical relations between data elements (such as exit velocity for stack parameters).

- Completeness cross-checks are performed between the plant, stack, process, and emission hierarchy levels of point source inventories. Each level should be associated with data at the next lower and higher level. For example process data should be subsidiary to corresponding stack information, and superior to associated emission data. Specific quality control checks are provided for each level of point, area, and mobile source inventories.

- Location checks, which are applied to determine that the specified political unit (e.g., county) is valid in each case, and that latitude and longitude coordinates (for point sources) are not reversed or missing. Political unit identifiers are checked against a list within IDA. When point-source latitude and longitude coordinates are missing, they are currently assigned to the pseudo-center of the appropriate county. The missing values are usually associated with smaller point sources. This assignment procedure can result in over-representation at the county center. Work is planned to better distribute point sources reported without geographic coordinates.

- Some emission inventories do not include sulfate (SO_4) emission data, which are important in modeling of particulate matter. The IDA can approximate SO_4 emission data by multiplying the source-category specific ratios of SO_4 to sulfur dioxide (SO_2) taken from the 1985 National Acid Precipitation Assessment Program (NAPAP) inventory, with SO_2 values in another inventory. The NAPAP inventory is considered to contain the best separate national modeling estimates of both SO_2 and SO_4 emissions at this time. If an inventory contains SO_4 data, this approximation feature is not used. The SO_4 estimator is optional in IDA. However, it is applied automatically in INPRO if no

SO_4 values are present. With this method, SO_4 estimates were supplied for the 1990 and 1995 U.S. inventories included with the initial Models-3 release.

- Occasionally an emission inventory contains an error in particulate matter emission values such that the fine fraction ($PM_{2.5}$) emissions exceed the value of the coarser fraction emissions (PM_{10}) of which they are a part. In the absence of more specific data, or information that the coarser particulate emission (PM_{10}) are in error, IDA automatically computes a new $PM_{2.5}$ value using the 1990 national inventory ratio of $PM_{2.5}$ to PM_{10} , which is expressed as $PM_{2.5} = .2411\ PM_{10}$.

- Point source stack emission parameters are essential to plume rise calculations in modeling. However, the stack parameters often have erroneous or missing values in emission inventories. In addition to range checks, IDA addresses the problem in two ways:

  (1) IDA examines point source files for consistency between stack flow rate, velocity, and diameter. The following relationship is used to correct erroneous velocity and flow values:

  $$F = V * 0.785398 * D^2 \qquad (4\text{-}1)$$

  where:
  F is flow (cubic feet/second)
  V is velocity (feet/second)
  D is stack diameter (feet)

  (2) In the event that all or most stack parameters are missing for a given point source, IDA supplies default values which are computed by SCC from other point sources in the same emission inventory.

4.2.2 The MEPPS Input Processor (INPRO)

The INPRO includes the MEPPS processors used to establish an emission study, the grid directory structure, and time-specific cases. These items are usually defined using the Models-3 Science Manager, specified through the Study Planner in the Models-3 framework, and passed to INPRO, unless MEPPS is being operated through the Tools Manager.

Import and Processing of Emission Inventories

The INPRO serves as the principal data access point for MEPPS. Two primary sets of data manipulations are accomplished in INPRO to prepare the data for further study-specific processing in MEPPS:

- The emission inventory data are subsetted and imported for the grid specified in the main MEPPS window and (if necessary) created in Science Manager. The emission data are subset from the user-selected emission inventory for the kinds of emission sources (point, area, mobile) specified by the user. The INPRO accepts inventories from IDA in the NET or IDA inventory formats (see Section 10.8 of the User Manual). The user must be sure that any aggregated (not hourly) data in the inventory for biogenic and mobile source emissions (other than vehicle miles traveled) are deleted from the inventory before use. Otherwise, MEPPS will double-count these emissions because hourly biogenic and mobile source emissions are modeled during processing.

- The INPRO imports meteorological data specific to the spatial domain and temporal case defined in Science Manager and selected in the MEPPS main window, provided that the meteorological data have been previously generated. The data come from the Mesoscale Meteorology Model 5 (MM5), via MCIP. The MCIP converts MM5 output to NetCDF IO/API files containing information needed by the rest of the Models-3 system (see Section 7.3 of this volume and Section 2.3.1 of the User Manual). In MEPPS, meteorology data are needed to model hourly biogenic and mobile source emissions (Sections 4.2.4.1 and 4.2.4.2). The MEPPS uses four of the files provided by MCIP, named MET_CRO_2D_ xx, MET_CRO_3D_ xx, GRID_DOT_2D_ xx, and MET_DOT_3D_ xx. The terms "CRO" and "DOT" refer to the cross and dot points of grids, respectively, and the suffixes “xx” are study specific identifiers. Refer to Chapter 12 for the details of the grid system definitions.

ROG-to-TOG Adjustment

Emission inventories may reflect different assumptions or methodologies with respect to volatile organic compound (VOC) gases. They may be reported as VOC, reactive organic gases (ROG) or total organic gases (TOG). It is typical to require TOG for air quality modeling, whereas the VOCs comprising organic gases in many regional inventories are reported as ROG. This occurs because some emission measurement techniques do not capture all of the discrete hydrocarbon compounds in the emission stream. Since the hydrocarbon speciation profiles are based on total organic compounds, the measured value of the hydrocarbon must be adjusted to account for the missing hydrocarbon components for the emission measurements that fail to capture the total organic emission stream. This adjustment is included as an option when importing an inventory using INPRO. The default is “yes” - perform the adjustment. More details are given in the speciation discussion in Section 4.2.5.

4.2.3 Processing Procedure

A detailed description of the processing procedure is given in Chapter 6 of the *Models-3 Volume 9B: User Manual*. Briefly, EMPRO receives point- and area-source emission data from INPRO for use in biogenic- and mobile-source emission modeling. The general sequence of processing for all of the emission data is (1) spatial allocation, (2) temporal allocation, and (3) chemical

speciation. There are some variations in processing between the general types (point, area, biogenic, mobile) of emission data because of the spatial and temporal resolution available and method of estimation. The gridded, temporally allocated and speciated data are passed to OUTPRO where they are merged into output files in the NetCDF I/O API format.

4.2.3.1 Spatial Allocation of Emission Data

The emission inventory data are usually provided by discrete point sources or by political units (typically counties in the United States). In order to prepare the data for use in air quality models and for analysis by grid-oriented visualization tools such as PAVE, the data must be spatially allocated (gridded) on a map projection and rectangular grid. The map coordinate system, grid position and spatial resolution are defined from windows in the Models-3 framework Science Manager (Sections 7.1 and 7.2 of the *Models-3 Volume 9B: User Manual*), although the actual grid creation is performed by the ARC/Info program. The MEPPS is capable of using Lambert Conformal, Mercator, Albers, and Universal Transverse Mercator (UTM) map projections; and several datums including perfect sphere, NAD83, and Clarke. However, in order to maintain consistency with gridded MM5 meteorology data, a spherical datum must be used. The radius used for Models-3 applications is 6370.997 kilometers.

Aside from the spherical datum restriction, the gridding processor allows development of a variety of emission grid systems which are used in different aspects of air quality modeling studies, including emission processing and in CMAQ. The gridding processor is written in the ARC® Macro Language (AML®) of the Arc/Info® geographic information system (GIS). Grids are used in MEPPS to spatially disaggregate or aggregate emission estimates, using land use/land cover data, and area source spatial surrogate data. Surrogate data are needed to spatially distribute emission data because the exact location of emission sources totaled for a county, for example, are seldom known. For example, census tract population data are of higher spatial resolution than county boundaries, and therefore population distribution could be assumed to be directly proportional to the spatial distribution of dry cleaning establishments. Land use cover data, detailed road network maps, and many other kinds of spatial data may be used as spatial surrogates to locate different source types of emissions, if GIS coverages of these data are available. At this time MEPPS is provided with GIS coverages for political boundaries and land cover for North America, and detailed population data and road networks for the United States.

The primary input to the gridding processor consists of user-supplied data that are entered into windows or chosen from a pick-list in the Coordinate System and Grid windows of the Models-3 Science Manager. These data define the grid projection system, the origin of the grid, cell size, etc., which is then generated by Arc/Info® through MEPPS. The primary output of the gridding processor for MEPPS is an ARC® coverage which consists of the intersection of the political boundaries and the fixed grid.

Use of the Arc/Info® GIS as the key component in the gridding processor allows substantial flexibility in the definition and use of grids and surrogate data. It also allows MEPPS to

incorporate visualization methods for quality control and for managing and querying of the spatial emission data.

To generate the emission modeling grid structure, a political boundaries (state and county boundaries) Arc/Info® coverage named "counties" must already exist in the exact map projection that is intended for the emission modeling grid structure. Accordingly the counties coverage provided with MEPPS is in the Lambert Conformal projection. If inconsistent projections are used, the gridding processor produces unpredictable results. The processor produces three files that are used elsewhere in EMPRO:

- A running history of emission modeling grid structure changes.
- A list of the geographic location of each grid cell in the emissions modeling grid structure.
- The Arc/Info® coverage of the emission modeling grid structure.

The gridding processor supports the following subset of Arc/Info® map projections:

- UTM (Universal Transverse Mercator)
- Lambert (Lambert Conformal Conic)
- Albers (Albers Conic Equal Area)
- Geographic (actual latitude and longitude coordinates rather than a projection)
- State (State Plane Coordinate System)

For more information about the Arc/Info® map projections, refer to the following:

- *ARC/INFO® User's Guide: Map Projections & Coordinate Management, Concepts and Procedures.*
- *ARC/INFO® Command References: ARC® Command References, Commands J-Z.*

The UTM map projection is a specialized application of the Transverse Mercator projection. It is limited to use between the latitudes of 84° North and 80° South, and divides the earth into 60 longitudinally-defined zones (UTM zones 1-60) with each zone spanning 6°of longitude. UTM zone 1 starts at 180° West longitude and ends at 174° West longitude. UTM zone 2 starts at 174° West longitude and ends at 168° West longitude, and so on around the globe. Shape, area, direction, and distance errors are all minimized if a study area is within a single zone; however, error increases rapidly as study areas cross UTM zone boundaries.

The Lambert map projection is a projection of the earth onto a cone intersecting the earth along two parallels called standard parallels (for example 30º North and 60º North). The projection is good for large scale (continental or smaller), middle latitude (between 45° North and 45° South) study areas. Shapes are maintained on a small scale (state or smaller), and large shapes (countries, continents) are minimally distorted. Area and distance are maintained near the standard parallels, but area is reduced between the standard parallels and increased beyond the

standard parallels; that is, the study area is accurately represented between the standard parallels. Direction is accurate within the entire study area. CMAQ is currently tested and used with a Lambert conformal projection.

The Albers map projection is suitable for study domains where the east-west extent is greater than the north-south extent. Shape is minimally distorted near the standard parallels as long as the study domain's east-west extent is greater than the study domain's north-south extent. Area is accurate within the study domain. Direction is accurate only at the standard parallels and minimally distorted between the standard parallels. If the study area is in the middle latitudes (45° North to 45° South), distances are minimally distorted at and between the standard parallels. If the study area falls outside of the middle latitudes, distance error increases rapidly as the poles are approached.

The Geographic system is not a true map projection; instead it is a global reference system. It is supported as a map projection because geographic positioning (latitude and longitude) is the most widely used method of map location. The origin of the geographic global reference system is at 0° longitude (Meridian of Greenwich) and 0° latitude (equator). Directions in the northeast quadrant are measured in positive longitude degrees by positive latitude degrees. Directions in the northwest quadrant are measured in negative longitude degrees by positive latitude degrees. Directions in the southwest quadrant are measured in negative longitude degrees by negative latitude degrees. Directions in the southeast quadrant are measured in positive longitude degrees by negative latitude degrees.

The State system is also not a true map projection; instead it is a specialized coordinate system for the United States, Puerto Rico, and the United States Virgin Islands. The State system divides the aforementioned areas into a total of 120 zones of varying sizes. The map projection is inherent in each zone. The three map projections that are used in the State system are the Lambert Conic Conformal (for zones with where the east-west extent is greater than the north-south extent), Transverse Mercator (for zones where the north-south extent is greater than the east-west extent), and Oblique Mercator (used only for the Alaska Panhandle). Direction, distance, area, and shape errors vary with the map projection inherent in each zone; however, the zones have been designed so that error is reduced or eliminated as long as the study area falls entirely within a state plan zone.

The spatial allocation process grid description file (*$EMS_GRD/grd_desc.in*) references numerous data items that are used by the Grid Definition Model to prepare the emissions modeling grid structure. Table 4-2 lists the run description file data items that affect processing in the Grid Definition Model.

Table 4-2. Data Items That Affect the Gridding Processor

Variable Name	Menu Identifier	Type	Example	Description
gridid	Grid Id:	C	grid_a	directory name and grid identifier
griddesc	Description:	C	Tutorial 36km Resolution Grid	descriptive text for the emissions modeling grid
cell_loc	Cell Location: (S,E)	C	SOUTHWEST	location on/in the grid cell from which to make measurements (NORTH, NORTHEAST, EAST, SOUTHEAST, SOUTH, SOUTHWEST, WEST, NORTHWEST, CENTER)
utmzn	UTM zone: (S,E)	N	10	UTM zones for which the emissions modeling grid exists (1-60)
utmxorig	Origin X direction: (S,E)	N	-108000	southwest x corner origin (measured from the origin of the projection) of the emissions modeling domain (meters)
utmyorig	Origin Y direction: (S,E)	N	-1080000	southwest y corner origin (measured from the origin of the projection) of the emissions modeling domain (meters)
cellsizx	Cell size X direction: (S,E)	N	36000	x grid cell size (meters)
cellsizy	Cell size Y direction: (S,E)	N	36000	y grid cell size (meters)
xcells	Number of cells X direction: (S,E)	N	21	number of grid cells in the x direction
ycells	Number of cells Y direction (S,E)	N	21	number of grid cells in the y direction
zcells	Number of cells Z direction: (S)	N	10	number of grid cells in the z direction (currently not used by ARC/INFO)
projectn	Name: (S,E)	C	LAMBERT	projection name (LAMBERT, UTM, ALBERS, STATE, GEOGRAPHIC)

Table 4-2. Data Items That Affect the Gridding Processor

Variable Name	Menu Identifier	Type	Example	Description
projunit	Units: (S,E)	C	METERS	units used to make measurements in the selected projection (METERS, FEET, DD [decimal degrees])
xshift	X-shift: (E)	N	0.0	constant value to add to x input coordinates (value in *projunit* – typically 0.0)
yshift	Y-shift: (E)	N	0.0	constant value to add to y input coordinates (value in *projunit* – typically 0.0)
projzone	UTM zone: (S,E)	N	16	State Plane or UTM zone (used only when *projectn* is STATE or UTM -- see *ARC Command References, Commands J-Z; Table PROJECT-3 and Table PROJECT-4* for valid values)
fipszone	FIPS zone for state plane projection: (E)	N	3701	FIPS code for State Plane zone (used only when *projectn* is STATE -- see *ARC Command References, Commands J-Z; Table PROJECT-5* for valid values)
datum	Datum conversion name for projection: (S,E)	C	MM5 (Perfect sphere)	datum upon which input coordinates are based (used only when *projectn* is STATE -- NAD27, NAD83, UNKNOWN)
p_1sp_dd	1st standard parallel DD: (S,E)	N	30	degree of first standard parallel (only for *projectn* ALBERS or LAMBERT)
p_1sp_mm	1st standard parallel MM: (S,E)	N	0	minutes of first standard parallel (only for *projectn* ALBERS or LAMBERT)
p_1sp_ss	1st standard parallel SS: (S,E)	N	0.00	seconds of first standard parallel (only for *projectn* ALBERS or LAMBERT)
p_2sp_dd	2nd standard parallel DD: (S,E)	N	60	degrees of second standard parallel (only for *projectn* ALBERS or LAMBERT)

Table 4-2. Data Items That Affect the Gridding Processor

Variable Name	Menu Identifier	Type	Example	Description
p_2sp_mm	2nd standard parallel MM: (S,E)	N	0	minutes of second standard parallel (only for *projectn* ALBERS or LAMBERT)
p_2sp_ss	2nd standard parallel SS: (S,E)	N	0.00	seconds of second standard parallel (only for *projectn* ALBERS or LAMBERT)
p_cen_dd	Central meridian DD: (S,E)	N	-90	degrees of central meridian of projection (only for *projectn* ALBERS or LAMBERT)
p_cen_mm	Central meridian MM: (S,E)	N	0	minutes of central meridian of projection (only for *projectn* ALBERS or LAMBERT)
p_cen_ss	Central meridian SS: (S,E)	N	0.00	seconds of central meridian of projection (only for *projectn* ALBERS or LAMBERT)
p_lpo_dd	Latitude of projection origin DD: (S,E)	N	40	degrees of latitude from projection origin (only for *projectn* ALBERS or LAMBERT)
p_lpo_mm	Latitude of projection origin MM: (S,E)	N	0	minutes of latitude from projection origin (only for *projectn* ALBERS or LAMBERT)
p_lpo_ss	Latitude of projection origin SS: (S,E)	N	0.00	seconds of latitude from projection origin (only for *projectn* ALBERS or LAMBERT)
p_f_east	False easting: (E)	N	0.0	false easting (only for *projectn* ALBERS or LAMBERT -- meters)
p_fnorth	False northing: (E)	N	0.0	false northing (only for *projectn* ALBERS or LAMBERT -- meters)

Variable Name refers to the name as it is found in the SAS® data set *run_desc.ssd01* which can be found in the directory referenced by the UNIX environment variable *EMS_RUN* (see *Models-3 Volume 9B: User Manual*, Chapter 6). Menu Identifier refers to the descriptive text found on the grid definition window in Science Manager (S) or the EMPRO Grid Processor window (E)

within MEPPS. Type refers to the variable type -- N is a numeric variable, and C is a character variable. Example gives an example of what might be entered for each data item. Description provides descriptive text about the data item, supported units, and a list of valid values that each data item recognizes -- valid values and units are listed in parentheses.

4.2.3.2 Temporal Allocation of Emission Data

Emission data that are based on annual, seasonal, weekly, or daily values must be temporally allocated (usually disaggregated) to hourly data for compatibility with the time scale of episodic air quality modeling. Generally, this procedure applies to regional inventories of point- and area-source emission data. Modeled emission data, such as biogenic- and mobile-source emissions are generated as hourly data for the time period of interest. Allocation of emission data from time periods greater than hourly (e.g., annual total, monthly total, weekly total), to hourly data is accomplished by use of seasonal, monthly, weekly, and daily diurnal temporal allocation factors to translate the data to daily total emission values. The daily values are then transformed into emission values for each hour of a typical day by using user-supplied or default temporal allocation profiles. The profiles assign proportions of the total daily emissions to each of the 24 hours of a typical day. Profiles are ideally source or source-category specific, but often are used for a range of similar source categories because of limited data on source category temporal variability. The majority of diurnal temporal source profiles have been developed for point sources, since more detailed reporting and monitoring exist for point sources, particularly large point sources, than for area sources which are spatially diverse and variable. Consequently are area source temporal allocation profiles tend to be less detailed and specific that point source temporal allocation profiles. Most of the temporal profiles used as defaults in MEPPS, were developed for the National Acid Rain Precipitation Assessment Program (NAPAP) (Fratt et al., 1990) and used in FREDS, with some more recent supplements (Moody et al., 1995).

In the EMPRO module of MEPPS, temporal allocation of point and area source category emission data is performed after spatial allocation of data in each main processor (point, area, biogenic, and mobile) and prior to speciation (see Chapter 6 of the Models-3 User Manual). This is transparent when running from Study Planner. If running in MEPPS under Tools Manager, the user may enter source category or source-specific daily or diurnal hourly temporal allocation data, or elect to use profiles computed by EMPRO (procedure described in the following sections) or use temporal allocation profiles based on those developed for use in the FREDS processors as supplemented. If a combination of emission inventory data at different temporal resolutions is used, EMPRO uses the most time-resolved (specific) data first, filling in with less time-specific data and applying temporal profiles as needed. If hourly, daily, and annual emission data are selected, EMPRO will provide hourly emission values taken from available data in the following order:

- Loading of hourly diurnal emission inventory (including Continuous Emission Monitoring (CEM) data);
- Loading and gridding of day-specific (daily) emission inventory data;

- Computing hourly emission data from annual or other longer-term emission inventory data.

Further details concerning temporal allocation are discussed as part of the following descriptions of the basis for processing each basic type of emission source.

4.2.3.3 Point Source Emission Data Processing

The point-source emission processor prepares gridded, temporally allocated point-source emission estimates suitable for speciation and reformatting for input to Models-3 framework for air quality modeling (e.g., CMAQ) (see Chapter 6 of the Models-3 User Manual). As previously indicated, the point-source emission processor does not compute basic emission estimates using emission factors and source-specific information. Instead, it reduces annual, point-source emission estimates to hourly, point source emissions estimates, unless the user is able to provide hourly emission data.

The point-source emission processor begins by establishing study-specific foundation emission estimates taken by INPRO from an user-specified emission inventory database. Foundation estimates (referred to as Foundation Files in MEPPS) are the basic annual emission inventory files imported to a processor (point, area, or mobile source) after quality control corrections have been applied and the data have been reduced to cover the study area only. After a point-source foundation file has been created, the processor spatially allocates the emission data into the spatial allocation grid structure, temporally allocates the emission estimates, and updates the hourly emission estimates derived from the foundation annual inventory with day-specific hourly emission estimates or hourly CEM data (if available). Usually, the point source-specific emission data are processed to files corresponding to the major hierarchical point-source data elements (i.e., Facility, Stack, Device, and Process), and translated to SAS® data sets.

Hourly emission estimates are computed using data from one of the following:

- Gridded emission estimates derived from annual emission inventory data by applying factors from source category-specific temporal allocation profiles
- Day and source-specific hourly emission data provided by the user
- Source-specific hourly CEM data.

Typically, the primary inputs to the point-source processor are the foundation emission annual estimates which are supplemented by available day-specific emission estimates. The primary output of the processor is the spatially and temporally allocated emission estimates.

<u>Computation of Point Source Emission Estimates</u>

The point-source emission processor treats emission estimates that have been prepared on one of the following bases: annual average; average day; or day-specific.

Day-Specific Emissions Estimates

Day-specific emission estimates are not computed by the MEPPS EMPRO point source processor. The user must supply any available day-specific emission estimates to the processor. Because day-specific emission estimates are more representative of actual conditions, they replace the hourly emission estimates derived from disaggregated annual emission data, when available. Day-specific emission data formats are made consistent with the internal formats of the SAS® data sets derived from other (e.g., annual) point-source emission data when imported through IDA.

CEM Hourly Emission Data

The CEM data are a subset of hourly emission data derived from continuous air pollutant concentration monitors attached to components of specific facilities, usually boilers or stacks of large point sources such as electric utilities. The data elements included are hourly emission rates for Carbon Monoxide (CO), nitrogen oxide, (NOx), and sulfur dioxide (SO_2). The CEM emission data are treated as hourly data imported to MEPPS via IDA. Electric utility CEM data are identified by specific source using their ORIS (Office of Regulatory Information Systems) identification number and are mapped to the corresponding point source identification number from an emission inventory. The CEM data are read in for a specified grid domain and day from a CEM dataset and substituted for hourly emission data derived from annual data. The CEM emission data are used in the format of data available for electric utility emissions provided by the U.S. EPA Acid Rain Division. The Acid Rain Division has electric utility CEM data for the United States for 1995 and 1996.

Spatial Allocation

Point sources are spatially allocated to an emission modeling grid by the geographic (latitude and longitude, UTM position) coordinates of a stack or by the geographic coordinates of the facility. The point-source emission data processor prepares an ASCII file of point-source identifiers and point-source geographic coordinate locations. The processor reads the ASCII file that was generated by the location processor, generates the appropriate ARC/INFO® coverages, and prepares two ASCII files:

- A file which contains point source identifiers and grid cell location; and
- A file which contains point-source identifiers and latitude/longitude coordinates. The process of assigning grid coordinates to point sources is an ARC/INFO® function; therefore, the underlying procedure follows the user documentation and proprietary code for the ARC/INFO® software.

Temporal Allocation

The EMPRO temporally allocates (produces hour-by-hour) foundation file emission estimates within each main emission processor (point, area, biogenic, and mobile emissions) based on

operating schedule data that are provided in one of two ways. The operating schedule data may be passed into the MEPPS EMPRO module via an ASCII foundation file, which corresponds with the segment (process) level of point source inventory information. For point sources, the temporal factors may be assigned by the user at the segment (process) level of the EMPRO point source hierarchy. The hierarchy is closely aligned with that of regional emission inventories. Temporal allocation factors may be also be applied at the device level in the facility, stack, device hierarchy. Alternatively, default source-category-specific temporal allocation factors may be selected. These factors were used in a MEPPS predecessor, FREDS, and are referred to as FREDS temporal allocation factors. The point source hierarchy for temporal allocation factors in FREDS is: plant, point, temporal factors. Source-specific temporal allocation factors are typically not available for large regional modeling domains. Consequently, the default temporal allocation factors are commonly used in regional modeling, perhaps more than 90 percent of the time. Note that EMPRO temporally allocates foundation file emission estimates, but not day-specific emissions estimates since the latter are entered on an hour-by-hour basis.

EMPRO provides a variety of methods for identifying operating schedule data:

- Seasonal throughput fractions (winter [Dec, Jan, Feb], spring [Mar, Apr, May], summer [Jun, Jul, Aug], and fall [Sep, Oct, Nov])
- Hours per year in operation
- Days per year in operation;
- Weeks per year in operation;
- Days per week in operation; and
- Hours per day in operation.

Any, none, or all of the operating schedule data can be supplied. If no operating schedule data are supplied, EMPRO uses a default continuous operating schedule of 24 hours per day, 7 days per week, and 52 weeks per year; otherwise, EMPRO filters through a hierarchy of the operating schedule data to determine how to compute the temporal factors:

- Weekly temporal factor;
- Daily temporal factor; and
- 24 hourly temporal factors.

To determine the weekly temporal factor, EMPRO determines the number of days in the year of interest and divides that value by 7 days per week. For example, in a leap year, there are 29 days in February; therefore, the weekly temporal factor is 366 days/year ÷ 7 days/week).

EMPRO computes a daily temporal factor through a lookup table based on the value of average 8-hour work days (days per week in operation) which is passed into MEPPS through the ASCII foundation files. To determine the daily temporal factor, EMPRO examines the values for days, hours per year (houryear), days per year (dayyear), and weeks respectively. If days has a valid value, EMPRO takes no further action to determine the days per week in operation for the source.

If days does not have a valid value, EMPRO attempts to assign an operation code value to days by examining houryear, dayyear, and weeks respectively:

- houryear (hours per year in operation)

  if houryear > 0 and houryear <= 850 then days = 2,
  if houryear > 850 and houryear <= 1250 then days = 3,
  if houryear > 1250 and houryear <= 1670 then days = 4,
  if houryear > 1670 and houryear <= 2100 then days = 5,
  if houryear > 2100 and houryear <= 2500 then days = 6,
  if houryear > 2500 then days = 7;

- dayyear (days per year in operation)

  if dayyear > 0 and dayyear <= 110 then days = 2,
  if dayyear > 110 and dayyear <= 160 then days = 3,
  if dayyear > 160 and dayyear <= 210 then days = 4,
  if dayyear > 210 and dayyear <= 260 then days = 5,
  if dayyear > 260 and dayyear <= 315 then days = 6,
  if dayyear > 315 then days = 7;

- weeks (weeks per year in operation)

  if weeks > 0 and weeks <= 7 then days = 1,
  if weeks > 7 and weeks <= 13 then days = 2,
  if weeks > 13 and weeks <= 19 then days = 3,
  if weeks > 19 and weeks <= 26 then days = 4,
  if weeks > 26 and weeks <= 33 then days = 5,
  if weeks > 33 and weeks <= 39 then days = 6,
  if weeks > 39 then days = 7.

EMPRO computes an hourly temporal factor through a lookup table based on the value of hours (hours per day in operation) which is passed into EMPRO through the ASCII foundation files. If hours has a valid value, the value is used and no further action is taken to determine the hours per day in operation for the source. If hours does not have a valid value, EMPRO attempts to assign a value to hours by examining houryear, dayyear, and weeks respectively, using the above tables. If houryear, dayyear, or weeks has a valid value, then hours is assigned a value of 8, again based on an average work day of 8 hours. If hours or days cannot be assigned through the method described above, operation is assumed to be continuous and hours is assigned a value of 24, and days is assigned a value of 7. The following calculations are performed.

$$week\_fac = daysinyear / 7 \quad (4\text{-}2)$$

$$day\_sum^{d} = \sum dy\_act_{i}^{d},\ i = 1,\ldots 7 \quad (4\text{-}3)$$

$$day\_fac_i = dy\_act_i^d / day\_sum^d,\ i = 1,... 7 \quad (4\text{-}4)$$
$$hour\_sum^h = \sum hr\_act_i^h,\ i = 1, ...24 \quad (4\text{-}5)$$
$$hrprof_i = hr\_act_i^h / hour\_sum^h,\ i = 1,... 24 \quad (4\text{-}6)$$

where week_fac is the weekly temporal factor
daysinyear is the number of days in the year (365 or 366)
day_sum is the total relative activity for the week
dy_act is an array that contains relative daily activities
day_fac is the day of week temporal factor
hour_sum is the total relative activity for the day
hrprof is an array of hourly temporal factors
hr_act is an array that contains relative hourly activities
d is an index indicating which days per week in operation code (days) to use
h is an index indicating which hours per day in operation code (days) to use
i is the integer count that applies (e.g., 7 days or 24 hours)

EMPRO uses the temporal factors to allocate emission estimates to hourly values. Application of the temporal factors depends on the temporal basis (annual average, day-specific, average day) that emissions estimates were input to EMPRO.

- if the temporal basis code estt = "AA" (annual average) then

$$hremis_i = aceekg/(week\_fac* day\_fac * hrprof_i),\ i = 1,... 24 \quad (4\text{-}7)$$

where hremis is the array of gridded, hourly emissions estimates (NO_X, TOG, CO, etc) (mass)
aceekg is the emission estimates (mass)
week_fac, day_fac, and hrprof are the weekly, daily and hourly temporal factors, respectively, computed by EMPRO

- if the temporal basis code estt = "AD" (average day) and (week_fac = 0 or day_fac = 0) then

$$hremis_i = 0.0,\ i = 1,... 24 \quad (4\text{-}8)$$

- if the temporal basis code estt = "AD" (average day) and not (week_fac = 0 or day_fac = 0) then

$$hremis_i = aceekg * hrprof_i,\ i = 1,... 24 \quad (4\text{-}9)$$

- if the temporal basis code estt = "DS" (day-specific) then

$$hremis_i = aceekg * prof_i,\ i = 1,... 24 \quad (4\text{-}10)$$

where prof is an array of day-specific, hourly temporal factors

4.2.3.4 Area Source Emission Data Processing

The area-source emission data processor prepares area-source emission estimates for speciation (lumped-model or discrete speciation) and reformatting for input to CMAQ or other Models-3 framework components. The area-source processor does not compute emission estimates from fundamental emission data. It reduces annual, county-wide emission estimates to emissions on an hourly, grid cell-by-grid cell basis. Most of the area source emission data processor is written in the SAS® programming language. The area-source spatial surrogates allocation component of the processor is written in the ARC® Macro Language (AML®). The primary inputs to the processor are the area-source emission estimates for the spatial domain of interest, and day-specific emission estimates (if available). The primary outputs are the spatially allocated, temporally resolved, emission estimates.

The processor begins with an area-source emission data base, extracted by INPRO from an emission inventory as an ASCII file and automatically converted to a SAS® file. The area-source processor updates the estimates with any available day-specific estimates, spatially allocates the emissions into the emission modeling grid, and temporally allocates the criteria emissions.

Emission Data Processing

This section discusses how area-source emission estimates are read into, manipulated by, and quality-assured by the area-source emission data processor. References are made to MEPPS source code where necessary to provide further details concerning area source emission allocation.
The processor uses county-wide area-source emission estimates, that have been prepared externally as part of an emission inventory, to produce spatially allocated, temporally resolved, pollutant emission estimates. To the extent that the inventory used includes small point sources in area source estimates, they are treated as area sources. All data provided as point sources, regardless of magnitude, are processed as point sources in EMPRO. The area-source emission data processor accommodates area-source emission estimates that have been prepared on the following bases: annual average; average day; or day-specific.

Day-specific emission data enter the area-source emission data processor during the temporal allocation step. Day-specific emission data are not computed by EMPRO. Like the foundation file emissions estimates, day-specific emission estimates are supplied from an external source to the emissions modeler. The day-specific emissions estimates replace the area-source emission estimates derived from annual inventory data because day-specific emission data are more representative of actual conditions.

Day-specific area-source emission estimates are summed to a daily total so that they are consistent with the internal formats of the SAS® data sets that maintain the other (e.g., derived

from annual emission inventories) area-source emissions estimates, which are passed to EMS-95 on an hourly basis.

Spatial Allocation

Area-source emission estimates are allocated to a modeling domain through the application of spatial surrogates. In general, surrogates approximate the value of unknown quantities. For example, population can be used to estimate the number of gasoline service stations. A spatial surrogate not only helps estimate the value of an unknown quantity, but a spatial surrogate also helps locate the unknown quantity.

For each spatial surrogate, it is necessary to specify what data (categories of land use/land cover, population counts, housing counts, etc.) contribute to the surrogate. In EMPRO, county area, land cover, population (census), Federal Highway Administration major roadway, and TIGER/LINE roadway data for the United States are provided as ARC® coverages for use as surrogates. Others may be added by providing ARC® coverages generated external to MEPPS. County area, and less detailed population and land cover coverages are provided for Canada and Mexico. Each area source category must be assigned a unique spatial surrogate value by grid cell. After the appropriate files have been populated, EMPRO grids the necessary data sets according to the requirements of the user-defined spatial surrogates. Each area source category (asct) which has been assigned to a spatial surrogate (k) can be allocated to grid cells (l, m) through the application of Equation 4-11.

$$acee_{i,j,k',l,m} = acee_{i,j,k'} * ratio_{i,j,k,l,m} \quad (4\text{-}11)$$

where i is the index on states
j is the index on counties within the states
k is the spatial surrogate index
k' is the area source category index (directly related to k)
l is the x cell index
m is the y cell index
acee is the county-wide area source emissions estimate (mass)
ratio is the gridded surrogate ratio by state/county/surrogate/cell

Each surrogate is computed through the application of Equations 4-12 and 4-13.

$$surtot_{i,j,k} = \Sigma_l \Sigma_m \ attribute_{i,j,k,l,m} \quad (4\text{-}12)$$

$$ratio_{i,j,k,l,m} = attribute_{i,j,k,l,m} / surtot_{i,j,k} \quad (4\text{-}13)$$

where:
i is the index on states
j is the index on counties within the states
k is the spatial surrogate index
l is the x cell index

m is the y cell index
surtot is the total value of a surrogate within specified (indexed) states and counties
attribute is the gridded value of the surrogate attribute by state/county/surrogate/cell
ratio is the gridded surrogate ratio for specified (indexed) states/counties/surrogates/cells

In the case of census data or other area-based or length-based surrogate information, it is necessary to area-apportion or length-apportion the surrogate (such as population or housing) information prior to aggregation to the cell level. This is because the locale of interest crosses cell boundaries. The assumption is that the surrogate information (such as population or housing) has a constant density across the locale (in the case of population or housing data, a constant density across the census tract). Therefore, in some cases, it is necessary to apply Equations 4-14 through 4-16 prior to the application of Equations 4-12 and 4-13.

$$arlg\_tot_{i,j,k} = \Sigma_l \Sigma_m \, arealeng_{i,j,k,l,m} \quad (4\text{-}14)$$

$$ap\_ratio_{i,j,k,l,m} = arealeng_{i,j,k,l,m} / arlg\_tot_{i,j,k} \quad (4\text{-}15)$$

$$attribute_{i,j,l,m} = attribute_{i,j,k} * ap\_ratio_{i,j,k,l,m} \quad (4\text{-}16)$$

where i is the index on states
j is the index on counties within the states
k is the locale of interest index (such as census tract or roadway)
l is the x cell index
m is the y cell index
arlg_tot is the total area or length of a locale of interest within specified (indexed) states and counties
arealeng is the gridded value of the specified (indexed) locale of interest by state/county/surrogate/cell
ap_ratio is the gridded ratio of the locale of interest specified (by indices) states/counties/locales/cell
attribute is the surrogate data (population, road length, etc.) for the area specified by indices.

As a check for Equations 4-14 through 4-16, the following must be true:

$$\Sigma_i \Sigma_j \Sigma_k \, ratio_{i,j,k} = 1.0 \quad (4\text{-}17)$$

Temporal Allocation

Temporal allocation of area source emission data is performed in an identical manner as described for point source processing in Section 4.2.3.3, although it is almost always necessary to use default temporal allocation profiles. Please refer to that section for a discussion of temporal allocation of area sources.

4.2.4 Modeled Emission Data

Emission data from available emission inventories are spatially and temporally allocated as described in the preceding paragraphs. Many anthropogenic area and point sources of emissions vary little or predictably with time, and can reasonably be disaggregated for regional modeling. However, some emission data are highly variable, diurnally and seasonally, because they are dependent on environmental variables, such as temperature, humidity, and solar insolation. It is more accurate to model these kinds of emissions on an hourly basis for direct use in episodic air quality modeling. The two principal kinds of sources for which hourly emission data are normally modeled are mobile sources and biogenic sources. In both cases, MEPPS takes hourly meteorological data from MCIP output derived from MM5.

4.2.4.1 Biogenic Emissions

Hourly biogenic emission rates for biogenic VOC compounds (including isoprenes, monoterpenes, and soil NO) for each grid cell are estimated using the Biogenic Emission Inventory System, Version 2 (BEIS-2) within MEPPS. In order to estimate biogenic emissions for modeling, it is necessary to apply biogenic emission and biomass factors to a geographic distribution of land cover. The BEIS-2 was developed to fill this need separately from Models-3 as an improvement on BEIS-1 (Pierce et al., 1990; Geron et al., 1994), and has been used in conjunction with different air quality modeling systems, including the Regional Acid Deposition Model (RADM) (Pierce et al., in press), the Regional Oxidant Model (ROM), and now Models-3 CMAQ. Additional information concerning BEIS-2 can be found in the Emission Inventory Improvement Program report on Biogenic Sources Preferred Methods (EIIP, 1996) and Pierce et al. (1998). The BEIS-2 model applies emission flux factors specific to tree genera and agricultural crop types by geographic area for biogenic emission species in accordance with equation 4-18.

$$ER_i = \sum_j [A_j * EF * F_{ij}(S,T)] \qquad (4\text{-}18)$$

where: ER is the emission rate (in grams/sec/model cell)
i is the chemical species (e.g., isoprene, monoterpene)
j is the vegetation type
A is the vegetation area (meter^2) in a grid cell
EF is the emission factor (micrograms/gram of leaf biomass/hour), and
$F_{ij}(S,T)$ is an environment factor to account for solar radiation S and leaf temperature T

Vegetation emission flux factors were adapted from those compiled by Geron et al. (1994) for 77 tree genera. Emission flux factors for 16 agricultural crops were taken primarily from Lamb et al (1993), and the emission factors applied to 34 land cover types are from the work of Guenther et al. (1994). Emission flux factors by land cover type are used principally for Canada and the western United States where genus-level forest cover and agricultural crop data were not available. Biogenic emission flux factors for summer and winter conditions are given in Table 4-3 and Table 4-4, respectively. The vegetation classes are taken from the Biogenic Emission Land Use Database (BELD) (Kinnee et al., 1997), which in turn is drawn from other land cover data sets, with an emphasis on forest and agricultural land cover. Spatial resolution of the raw (original) land cover data is at the county-level for the United States and sub-province level for Canada. Emission flux factors are based on full leaf summer conditions normalized to leaf or soil temperatures of 30ºC and photosynthetically active radiation (PAR) of 1000 micromoles/m^2/sec. For use in regional modeling, the mass of biogenic emissions are converted to moles by dividing the mass (grams-compound) by the molecular weight of the compound. The emission factors for tree genus and agricultural vegetation, and used in the Models-3 application of BEIS-2 are compiled by Pierce et al. (1998).

Table 4-3. Summer Biogenic Emission Flux Factors (μg-compound $m^{-2}hr^{-1}$) for Principal Biogenic Compounds by Vegetation Category

Vegetation or Land Cover Code	Isoprene	Terpene	Other VOCs	NO	Leaf Area Index (m^2 m^{-2})	Description
Abie	170.0	5100.0	2775.0	4.5	7	Abies (fir)
Acac	79.3	2380.0	1295.0	4.5	5	Acacia
Acer	42.5	680.0	693.7	4.5	5	Acer (maple)
Aesc	42.5	42.5	693.7	4.5	5	Aesculus (buckeye)
Aila	42.5	42.5	693.7	4.5	5	Ailanthus
Aleu	42.5	42.5	693.7	4.5	5	Aleurites (tung-oil tree)
Alfa	19.0	7.6	11.4	12.8	0	Alfalfa
Alnu	42.5	42.5	693.7	4.5	5	Alnus (European alder)
Amel	42.5	42.5	693.7	4.5	5	Amelanchier (serviceberry)
Asim	42.5	42.5	693.7	4.5	5	Asimina (pawpaw)
Avic	42.5	42.5	693.7	4.5	5	Avicennia (black mangrove)
Barl	7.6	19.0	11.4	256.7	0	Barley
Barr	0.0	0.0	0.0	0.0	0	Barren

Table 4-3. Summer Biogenic Emission Flux Factors (μg-compound $m^{-2}hr^{-1}$) for Principal Biogenic Compounds by Vegetation Category

Vegetation or Land Cover Code	Isoprene	Terpene	Other VOCs	NO	Leaf Area Index (m^2 m^{-2})	Description
Betu	42.5	85.0	693.7	4.5	5	Betula (birch)
Borf	910.0	713.0	755.0	4.5	5	Boreal forest (Guenther*)
Bume	42.5	42.5	693.7	4.5	5	Bumelia (gum bumelia)
Carp	42.5	680.0	693.7	4.5	5	Carpinus (hornbean)
Cary	42.5	680.0	693.7	4.5	5	Carya (hickory)
Casp	42.5	42.5	693.7	4.5	5	Castanopsis (chinkapin)
Cast	42.5	42.5	693.7	4.5	5	Castanea (chestnut)
Casu	29750.0	42.5	693.7	4.5	7	Casuarina (Austl pine)
Cata	42.5	42.5	693.7	4.5	5	Catalpa
Cedr	79.3	1269.3	1295.0	4.5	7	Cedrus (Deodar cedar)
Celt	42.5	85.0	693.7	4.5	5	Celtis (hackberry)
Cerc	42.5	42.5	693.7	4.5	5	Cercis (redbud)
Cham	170.0	340.0	2775.0	4.5	7	Chamaecyparis (prt-orford cedar)
Citr	42.5	680.0	693.7	4.5	5	Citrus (orange)
Cnif	745.4	1366.6	993.9	4.5	9	BEIS conifer forest
Conf	1550.0	1564.0	1036.0	4.5	6	Conifer forest (Guenther)
Corn	0.5	0.0	0.0	577.6	0	Corn
Coru	42.5	680.0	693.7	4.5	5	Cornus (dogwood)
Coti	42.5	42.5	693.7	4.5	5	Cotinus (smoke tree)
Cott	7.6	19.0	11.4	256.7	0	Cotton
Crat	42.5	42.5	693.7	4.5	5	Crataegus (hawthorn)
Cswt	1050.0	660.0	770.0	0.2	2	Herbaceous Wetlands (Guenther)
Desh	65.0	94.5	56.7	57.8	0	Desert shrub (Guenther)
Dios	42.5	42.5	693.7	4.5	5	Diospyros (persimmon)

Table 4-3. Summer Biogenic Emission Flux Factors (μg-compound $m^{-2}hr^{-1}$) for Principal Biogenic Compounds by Vegetation Category

Vegetation or Land Cover Code	Isoprene	Terpene	Other VOCs	NO	Leaf Area Index (m^2 m^{-2})	Description
Euca	29750.0	1275.0	693.7	4.5	5	Eucalyptus
Fagu	42.5	255.0	693.7	4.5	5	Fagus (american beech)
Frax	42.5	42.5	693.7	4.5	5	Fraxinus (ash)
Gled	42.5	42.5	693.7	4.5	5	Gleditsia (honey locust)
Gord	42.5	42.5	693.7	4.5	5	Gordonia (loblolly-bay)
Gras	56.2	140.5	84.3	57.8	0	Grass
Gymn	42.5	42.5	693.7	4.5	5	Gymnocladus (KY coffeetree)
Hale	42.5	42.5	693.7	4.5	5	Halesia (silverbell)
Harf	8730.0	436.0	882.0	4.5	5	Hardwood forest (Guenther)
Hay	37.8	94.5	56.7	12.8	0	Hay
Ilex	42.5	85.0	693.7	4.5	5	Ilex (holly)
Jugl	42.5	1275.0	693.7	4.5	5	Juglans (black walnut)
Juni	79.3	476.0	1295.0	4.5	7	Juniperus (east. red cedar)
Lagu	42.5	42.5	693.7	4.5	5	Laguncularia (white mangrove)
Lari	42.5	42.5	693.7	4.5	5	Larix (larch)
Liqu	29750.0	1275.0	693.7	4.5	5	Liquidambar (sweetgum)
Liri	42.5	85.0	693.7	4.5	5	Liriodendron (yellow poplar)
Macl	42.5	42.5	693.7	4.5	5	Maclura (osage-orange)
Magn	42.5	1275.0	693.7	4.5	5	Magnolia
Malu	42.5	42.5	693.7	4.5	5	Malus (apple)
Meli	42.5	42.5	693.7	4.5	5	Melia (chinaberry)
Mixf	11450.0	1134.0	1140.0	4.5	5	Mixed forest (Guenther)
Moru	42.5	85.0	693.7	4.5	5	Morus (mulberry)
Mscp	7.6	19.0	11.4	12.8	0	Misc crops

Table 4-3. Summer Biogenic Emission Flux Factors (μg-compound $m^{-2}hr^{-1}$) for Principal Biogenic Compounds by Vegetation Category

Vegetation or Land Cover Code	Isoprene	Terpene	Other VOCs	NO	Leaf Area Index (m^2 m^{-2})	Description
Nmxf	10150.0	1100.0	850.0	4.5	5	Northern Mixed Forest (Guenther)
Nyss	5950.0	255.0	693.7	4.5	5	Nyssa (blackgum)
Oak	3108.3	255.5	894.2	4.5	6	BEIS oak forest
Oats	7.6	19.0	11.4	256.7	0	Oats
Odcd	2112.4	368.8	871.8	4.5	6	BEIS other deciduous forest
Ofor	56.2	140.5	84.3	4.5	0	Open forest
Oksv	7350.0	100.0	600.0	4.5	2	Oak Savannah (Guenther)
Ostr	42.5	42.5	693.7	4.5	5	Ostrya (hophornbeam)
Othe	56.2	140.5	84.3	57.8	0	Other (unknown, assume grass)
Oxyd	42.5	255.0	693.7	4.5	5	Oxydendrum (sourwood)
Pacp	55.0	79.8	47.9	35.3	0	Pasture crop land (Guenther)
Past	56.2	140.5	84.3	57.8	0	Pasture
Paul	42.5	42.5	693.7	4.5	5	Paulownia
Pean	102.0	255.0	153.0	12.8	0	Peanuts
Pers	42.5	255.0	693.7	4.5	5	Persea (redbay)
Pice	23800.0	5100.0	2775.0	4.5	7	Picea (spruce)
Pinu	79.3	2380.0	1295.0	4.5	3	Pinus (pine)
Plan	42.5	42.5	693.7	4.5	5	Planera (water elm)
Plat	14875.0	42.5	693.7	4.5	5	Platanus (sycamore)
Popu	29750.0	42.5	693.7	4.5	5	Populus (aspen)
Pota	9.6	24.0	14.4	192.5	0	Potato
Pros	42.5	42.5	693.7	4.5	5	Prosopis (mesquite)
Prun	42.5	42.5	693.7	4.5	5	Prunus (cherry)
Pseu	170.0	2720.0	2775.0	4.5	7	Pseudotsuga (douglas fir)

Table 4-3. Summer Biogenic Emission Flux Factors (μg-compound $m^{-2}hr^{-1}$) for Principal Biogenic Compounds by Vegetation Category

Vegetation or Land Cover Code	Isoprene	Terpene	Other VOCs	NO	Leaf Area Index (m^2 m^{-2})	Description
Quer	29750.0	85.0	693.7	4.5	5	Quercus (oak)
Rang	37.8	94.5	56.7	57.8	0	Range
Rhiz	42.5	42.5	693.7	4.5	5	Rhizophora (red mangrove)
Rice	102.0	255.0	153.0	0.2	0	Rice
Robi	5950.0	85.0	693.7	4.5	5	Robinia (black locust)
Rye	7.6	19.0	11.4	12.8	0	Rye
Sabl	5950.0	42.5	693.7	4.5	5	Sabal (cabbage palmetto)
Sali	14875.0	42.5	693.7	4.5	5	Salix (willow)
Sapi	42.5	42.5	693.7	4.5	5	Sapium (chinese tallow tree)
Sass	42.5	42.5	693.7	4.5	5	Sassafras
Scru	37.8	94.5	56.7	57.8	0	Scrub
Scwd	2700.0	349.0	651.0	31.2	2	Scrub woodland (Guenther)
Sere	14875.0	42.5	693.7	4.5	5	Serenoa (saw palmetto)
Shrf	10750.0	530.0	910.0	4.5	5	Southeast/Western Deciduous Forest
Smxf	17000.0	1500.0	1250.0	4.5	4	Southeast Mixed Forest
Snow	0.0	0.0	0.0	0.0	0	Snow
Sor	42.5	42.5	693.7	4.5	5	Sorbus (mountain ash)
Sorg	7.8	19.5	11.7	577.6	0	Sorghum
Soyb	22.0	0.0	0.0	12.8	0	Soybean
Spin	1460.0	1983.0	1252.0	4.5	3	Southern pine (Guenther)
Swie	42.5	42.5	693.7	4.5	5	Swietenia (W. Indies mahogany)
Taxo	42.5	1275.0	693.7	4.5	5	Taxodium (cypress)
Thuj	170.0	1020.0	2775.0	4.5	7	Thuja (W. red cedar)
Tili	42.5	42.5	693.7	4.5	5	Tilia (basswood)

Table 4-3. Summer Biogenic Emission Flux Factors (μg-compound $m^{-2}hr^{-1}$) for Principal Biogenic Compounds by Vegetation Category

Vegetation or Land Cover Code	Isoprene	Terpene	Other VOCs	NO	Leaf Area Index (m^2 m^{-2})	Description
Toba	0.0	58.8	235.2	256.7	0	Tobacco
Tsug	79.3	158.7	1295.0	4.5	7	Tsuga (Eastern hemlock)
Tund	2411.7	120.6	150.7	0.2	0	Tundra
Ufor	1988.7	663.7	920.0	4.5	0	BEIS urban forest
Ugra	56.2	140.5	84.3	57.8	0	BEIS urban grass
Ulmu	42.5	42.5	693.7	4.5	5	Ulmus (American elm)
Uoth	0.0	0.0	0.0	0.0	0	BEIS other urban (barren)
Urba	408.6	161.9	200.5	12.5	0	BEIS urban (.2 grass/.2 forest)
Utre	5140.0	1000.0	959.0	4.5	5	Urban trees (.5 Harf/.5 Conf)
Vacc	42.5	42.5	693.7	4.5	5	Vaccinium (blueberry)
Wash	5950.0	42.5	693.7	4.5	5	Washingtonia (fan palm)
Wate	0.0	0.0	0.0	0.0	0	Water
Wcnf	4270.0	1120.0	1320.0	4.5	5	W Coniferous Forest (Guenther)
Wdcp	2550.0	663.0	2053.0	8.7	3	Woodland/crop land (Guenther)
Wetf	3820.0	923.0	1232.0	0.2	5	Wetland forest (Guenther)
Whea	15.0	6.0	9.0	192.5	0	Wheat
Wmxf	5720.0	620.0	530.0	4.5	4	Western Mixed Forest (Guenther)
Wwdl	525.0	250.0	360.0	4.5	3	Western Woodlands (Guenther)

*Guenther references biogenic emission factors taken from Guenther et al. (1994) using AVHRR (Advanced Very High Resolution Radiometer) satellite imagery.

Table 4-4. Winter Biogenic Emission Flux Factors (μg-compound $m^{-2}hr^{-1}$) for Principal Biogenic Compounds by Vegetation Category

Vegetation or Land Cover Code	Isoprene	Terpene	Other VOCs	NO	Leaf Area Index (m^2 m^{-2})	Description
Abie	170.0	5100.0	2775.0	4.5	7	Abies (fir)
Acac	0.0	0.0	0.0	4.5	5	Acacia
Acer	0.0	0.0	0.0	4.5	5	Acer (maple)
Aesc	0.0	0.0	0.0	4.5	5	Aesculus (buckeye)
Aila	0.0	0.0	0.0	4.5	5	Ailanthus
Aleu	0.0	0.0	0.0	4.5	5	Aleurites (tung-oil tree)
Alfa	0.0	0.0	0.0	12.8	0	Alfalfa
Alnu	0.0	0.0	0.0	4.5	5	Alnus (European alder)
Amel	0.0	0.0	0.0	4.5	5	Amelanchier (serviceberry)
Asim	0.0	0.0	0.0	4.5	5	Asiminia (pawpaw)
Avic	42.5	42.5	693.7	4.5	5	Avicennia (black mangrove)
Barl	0.0	0.0	0.0	256.7	0	Barley
Barr	0.0	0.0	0.0	0.0	0	Barren
Betu	0.0	0.0	0.0	4.5	5	Betula (birch)
Borf	640.0	706.0	634.0	4.5	6	Boreal forest (AVHRR/G.*)
Bume	42.5	42.5	693.7	4.5	5	Bumelia (gum bumelia)
Carp	0.0	0.0	0.0	4.5	5	Carpinus (hornbean)
Cary	0.0	0.0	0.0	4.5	5	Carya (hickory)
Casp	0.0	0.0	0.0	4.5	5	Castanopsis (chinkapin)
Cast	0.0	0.0	0.0	4.5	5	Castanea (chestnut)
Casu	29750.0	42.5	693.7	4.5	7	Casuarina (Austl pine)

Table 4-4. Winter Biogenic Emission Flux Factors (μg-compound $m^{-2}hr^{-1}$) for Principal Biogenic Compounds by Vegetation Category

Vegetation or Land Cover Code	Isoprene	Terpene	Other VOCs	NO	Leaf Area Index (m^2 m^{-2})	Description
Cata	0.0	0.0	0.0	4.5	5	Catalpa
Cedr	79.3	1269.3	1295.0	4.5	7	Cedrus (Deodar cedar)
Celt	0.0	0.0	0.0	4.5	5	Celtis (hackberry)
Cerc	0.0	0.0	0.0	4.5	5	Cercis (redbud)
Cham	170.0	340.0	2775.0	4.5	7	Chamaecyparis (prt-orford cedar)
Citr	42.5	680.0	693.7	4.5	5	Citrus (orange)
Cnif	0.0	1353.0	835.0	4.5	9	BEIS conifer forest
Conf	1400.0	1548.0	870.0	4.5	6	Conifer forest (AVHRR, G.)
Corn	0.0	0.0	0.0	577.6	0	Corn
Coru	0.0	0.0	0.0	4.5	5	Cornus (dogwood)
Coti	0.0	0.0	0.0	4.5	5	Cotinus (smoke tree)
Cott	0.0	0.0	0.0	256.7	0	Cotton
Crat	0.0	0.0	0.0	4.5	5	Crataegus (hawthorn)
Cswt	1050.0	660.0	770.0	0.2	1	Herbaceous Wetlands (AVHRR, G.)
Desh	0.0	0.0	0.0	57.8	0	Desert shrub (AVHRR, G.)
Dios	0.0	0.0	0.0	4.5	5	Diospyros (persimmon)
Euca	29750.0	1275.0	693.7	4.5	5	Eucalyptus
Fagu	0.0	0.0	0.0	4.5	5	Fagus (american beech)
Frax	0.0	0.0	0.0	4.5	5	Fraxinus (ash)
Gled	0.0	0.0	0.0	4.5	5	Gleditsia (honeylocust)

Table 4-4. Winter Biogenic Emission Flux Factors (μg-compound $m^{-2}hr^{-1}$) for Principal Biogenic Compounds by Vegetation Category

Vegetation or Land Cover Code	Isoprene	Terpene	Other VOCs	NO	Leaf Area Index (m^2 m^{-2})	Description
Gord	0.0	0.0	0.0	4.5	5	Gordonia (loblolly-bay)
Gras	0.0	0.0	0.0	57.8	0	Grass
Gymn	0.0	0.0	0.0	4.5	5	Gymnocladus (KY coffeetree)
Hale	0.0	0.0	0.0	4.5	5	Halesia (silverbell)
Harf	0.0	371.0	185.0	4.5	3	Hardwood forest (AVHRR, G.)
Hay	0.0	0.0	0.0	12.8	0	Hay
Ilex	42.5	85.0	693.7	4.5	5	Ilex (holly)
Jugl	0.0	0.0	0.0	4.5	5	Juglans (black walnut)
Juni	79.3	476.0	1295.0	4.5	7	Juniperus (east. red cedar)
Lagu	42.5	42.5	693.7	4.5	5	Laguncularia (white mangrove)
Lari	0.0	0.0	0.0	4.5	5	Larix (larch)
Liqu	0.0	0.0	0.0	4.5	5	Liquidambar (sweetgum)
Liri	0.0	0.0	0.0	4.5	5	Liriodendron (yellow poplar)
Macl	0.0	0.0	0.0	4.5	5	Maclura (osage-orange)
Magn	42.5	1275.0	693.7	4.5	5	Magnolia
Malu	0.0	0.0	0.0	4.5	5	Malus (apple)
Meli	0.0	0.0	0.0	4.5	5	Melia (chinaberry)
Mixf	0.0	1077.0	581.0	4.5	4	Mixed forest (AVHRR, G.)
Moru	0.0	0.0	0.0	4.5	5	Morus (mulberry)
Mscp	0.0	0.0	0.0	12.8	0	Misc crops

Table 4-4. Winter Biogenic Emission Flux Factors (μg-compound $m^{-2}hr^{-1}$) for Principal Biogenic Compounds by Vegetation Category

Vegetation or Land Cover Code	Isoprene	Terpene	Other VOCs	NO	Leaf Area Index (m^2 m^{-2})	Description
Nmxf	175.0	1100.0	850.0	4.5	1	Northern Mixed Forest (AVHRR, G.)
Nyss	0.0	0.0	0.0	4.5	5	Nyssa (blackgum)
Oak	0.0	217.0	188.0	4.5	6	BEIS oak forest
Oats	0.0	0.0	0.0	256.7	0	Oats
Ocdf	0.0	313.0	183.0	4.5	6	BEIS other deciduous forest
Ofor	0.0	0.0	0.0	4.5	0	Open forest
Oksv	0.0	100.0	200.0	4.5	1	Oak Savannah (AVHRR, Guen)
Ostr	0.0	0.0	0.0	4.5	5	Ostrya (hophornbeam)
Othe	0.0	0.0	0.0	57.8	0	Other (unknown, assume grass)
Oxyd	0.0	0.0	0.0	4.5	5	Oxydendrum (sourwood)
Pacp	0.0	0.0	0.0	35.3	0	Pasture cropland (AVHRR, G.)
Past	0.0	0.0	0.0	57.8	0	Pasture
Paul	0.0	0.0	0.0	4.5	5	Paulownia
Pean	0.0	0.0	0.0	12.8	0	Peanuts
Pers	42.5	255.0	693.7	4.5	5	Persea (redbay)
Pice	23800.0	5100.0	2775.0	4.5	7	Picea (spruce)
Pinu	79.3	2380.0	1295.0	4.5	3	Pinus (pine)
Plan	0.0	0.0	0.0	4.5	5	Planera (water elm)
Plat	0.0	0.0	0.0	4.5	5	Platanus (sycamore)
Popu	0.0	0.0	0.0	4.5	5	Populus (aspen)
Pota	0.0	0.0	0.0	92.15	0	Potato

Table 4-4. Winter Biogenic Emission Flux Factors (μg-compound $m^{-2}hr^{-1}$) for Principal Biogenic Compounds by Vegetation Category

Vegetation or Land Cover Code	Isoprene	Terpene	Other VOCs	NO	Leaf Area Index (m^2 m^{-2})	Description
Pros	0.0	0.0	0.0	4.5	5	Prosopis (mesquite)
Prun	0.0	0.0	0.0	4.5	5	Prunus (cherry)
Pseu	170.0	2720.0	2775.0	4.5	7	Pseudotsuga (douglas fir)
Quer	0.0	0.0	0.0	4.5	5	Quercus (oak)
Rang	0.0	0.0	0.0	57.8	0	Range
Rhiz	42.5	42.5	693.7	4.5	5	Rhizophora (red mangrove)
Rice	0.0	0.0	0.0	0.2	0	Rice
Robi	0.0	0.0	0.0	4.5	5	Robinia (black locust)
Rye	0.0	0.0	0.0	12.8	0	Rye
Sabl	5950.0	42.5	693.7	4.5	5	Sabal (cabbage palmetto)
Sali	0.0	0.0	0.0	4.5	5	Salix (willow)
Sapi	0.0	0.0	0.0	4.5	5	Sapium (chinese tallow tree)
Sass	0.0	0.0	0.0	4.5	5	Sassafras
Scru	0.0	0.0	0.0	57.8	0	Scrub
Scwd	0.0	332.0	332.0	31.2	2	Scrub woodland (AVHRR, G.)
Sere	14875.0	42.5	693.7	4.5	5	Serenoa (saw palmetto)
Shrf	0.0	0.0	0.0	4.5	0	SE/W Deciduous Forest (AVHRR, G.)
Smxf	0.0	1500.0	500.0	4.5	2	SE Mixed Forest (AVHRR, G.)
Snow	0.0	0.0	0.0	0.0	0	Snow
Sorb	0.0	0.0	0.0	4.5	5	Sorbus (mountain ash)

Table 4-4. Winter Biogenic Emission Flux Factors (μg-compound $m^{-2}hr^{-1}$) for Principal Biogenic Compounds by Vegetation Category

Vegetation or Land Cover Code	Isoprene	Terpene	Other VOCs	NO	Leaf Area Index (m^2 m^{-2})	Description
Sorg	0.0	0.0	0.0	577.6	0	Sorghum
Soyb	0.0	0.0	0.0	12.8	0	Soybean
Spin	0.0	1963.0	1052.0	4.5	3	Southern pine (AVHRR, G.)
Swie	42.5	42.5	693.7	4.5	5	Swietenia (W. Indies mahogany)
Taxo	42.5	1275.0	693.7	4.5	5	Taxodium (cypress)
Thuj	170.0	1020.0	2775.0	4.5	7	Thuja (W. red cedar)
Tili	0.0	0.0	0.0	4.5	5	Tilia (basswood)
Toba	0.0	0.0	0.0	256.7	0	Tobacco
Tsug	79.3	158.7	1295.0	4.5	7	Tsuga (Eastern hemlock)
Tund	0.0	0.0	0.0	0.2	0	Tundra
Ufor	0.0	631.0	469.0	4.5	0	BEIS urban forest
Ugra	0.0	0.0	0.0	57.8	0	BEIS urban grass
Ulmu	0.0	0.0	0.0	4.5	5	Ulmus (American elm)
Uoth	0.0	0.0	0.0	0.0	0	BEIS other urban (barren)
Urba	0.0	154.0	102.0	12.5	0	BEIS urban (.2 grass/.2 forest)
Utre	700.0	960.0	528.0	4.5	6	Urban tree (.5 Harf/.5 Conf)
Vacc	0.0	0.0	0.0	4.5	5	Vaccinium (blueberry)
Wash	5950.0	42.5	693.7	4.5	5	Washingtonia (fan palm)
Wate	0.0	0.0	0.0	0.0	0	Water
Wcnf	3500.0	1120.0	1200.0	4.5	5	Western Coniferous Forest (AVHRR, G.)

Table 4-4. Winter Biogenic Emission Flux Factors (μg-compound $m^{-2}hr^{-1}$) for Principal Biogenic Compounds by Vegetation Category

Vegetation or Land Cover Code	Isoprene	Terpene	Other VOCs	NO	Leaf Area Index (m^2 m^{-2})	Description
Wdcp	0.0	630.0	1047.0	8.7	2	Woodland/cropland (AVHRR, G.)
Wetf	0.0	877.0	628.0	0.2	3	Wetland forest (AVHRR, G.)
Whea	0.0	0.0	0.0	192.5	0	Wheat
Wmxf	0.0	620.0	330.0	4.5	3	Western Mixed Forest (AVHRR, G.)
Wwdl	0.0	250.0	360.0	4.5	3	Western Woodlands (AVHRR, G.)

* AVHRR/G. references biogenic emission factors from Guenther et al (1994) which used land use classifications from Advanced Very High Resolution Radiometer (AVHRR) satellite imagery.

The BEIS-2 applies environmental correction factors to account for the effect of leaf temperature and visible solar radiation on isoprene (Pierce et al.,1998). Specifically:

$$I = I_s * C_L * C_T \quad (4\text{-}19)$$

where: I is the adjusted isoprene emission flux,
I_S is the isoprene emission flux standardized to leaf temperature 30°C and PAR of 1000 micromoles/m^2/sec.

The light adjustment factor C_L is estimated by:

$$C_L = (\alpha c_{L1} PAR) / \sqrt{(1+\alpha^2 PAR2)} \quad (4\text{-}20)$$

where: $\alpha = 0.0027$, and $C_{L1} = 1.066$ are empirically derived coefficients. The leaf temperature adjustment factor C_T is derived from laboratory data and is computed using the following formula:

$$C_T = (\exp[c_{T1}(T-T_s)/RT_sT])/ (1+\exp[c_{T2}(T-T_m)/RT_sT]) \quad (4\text{-}21)$$

where: $C_{T1} = 95{,}000$ J mol^{-1}
T_s is the standardized temperature (303°K),
R is the ideal gas constant (8.314 °K mol^{-1}),
$C_{T2} = 230{,}000$ J mol^{-1}, and

$T_m = 314^oK$.

PAR is computed as a function of height by:

$$PAR_z = PAR_0 (\exp[-0.42LAI_z]) \quad (4\text{-}22)$$

During March 1998, the factor used in BEIS-2 within Models-3 to convert solar radiation values from watts per square meter (W/m^2) to micromoles per square meter-second ($\mu m/m^2$-sec) was changed from 2.2982 to 2, based on Alados et al. (1996). This had the effect of reducing PAR by ~ 15 percent and isoprene emissions by ~ 5 percent based on limited simulation tests for the July 1995 ozone maximum period.

Emissions for VOCs other that isoprene are assumed to vary only as a function of leaf temperature in accordance with the following:

$$E = E_s * \exp[0.09 (T-T_s)] \quad (4\text{-}23)$$

where: E_s is the standardized emission flux for monoterpenes and other VOCs,
T is the leaf temperature in degrees Kelvin, and
T_s is the standardized temperature (303^oK).

The soil NO emission flux factors used in BEIS-2 were adapted from Williams et al. (1992). For temperatures greater than 0^oC, soil NO temperature corrections follow the formulation of Williams et al. As follows:

$$NO = NO_o * \exp[0.071(T-T_s)] \quad (4\text{-}24)$$

where NO is the adjusted soil NO emission flux,
NO_o is the emission flux standardized to a soil temperature T_s of 30^o C, and
T is the soil temperature.

NO emissions at temperatures less than 0^o C are set to zero. During March 1998, it was decided to cap the exponential increase of soil NO emissions with temperatures above 30^oC, based on the findings of Yienger and Levy (1995).

The inclusion of BEIS-2 into MEPPS biogenic emission modeling required creating an efficient connection such that BEIS-2 is easy to use from within MEPPS, and also so that the input and output data related to BEIS-2 can take advantage of MEPPS and Models-3 data handling and analysis features. The changes included:

- BEIS-2 is now automatically invoked from MEPPS or the Study Planner when the user requests that biogenic emission factors be calculated. It is not necessary to work directly with the BEIS-2 software.

- Solar radiation and temperature input files are not directly supplied by the user when BEIS-2 is run. These meteorological data are supplied automatically from MCIP files for the case (time period) specified, presuming that MM5 and MCIP have been run for that period.

- Within MEPPS, BEIS-2 can now use ARC-INFO® generated grids and use gridded surrogate data to disaggregate county-level data to grid cells.

- BEIS-2 results are in terms of hourly emissions per grid cell within Models-3.

- Biogenic emission data are subject to the extended quality control and reporting features in MEPPS, and visualization using the ARC-INFO® based GIS-View feature.

The MEPPS uses BEIS-2 by allowing the user to assume summer, winter seasons, or access frost data in order to allow for the seasonal change in vegetative biomass. For summer and winter conditions, vegetation genus and emission factors for isoprene, monoterpene, other biogenic VOC emissions, emission factors for NO, and the leaf area index (LAI) are provided based on the work of Geron et al. (1994). Frost data include the federal identification protocol (FIPS) codes by state and county along with the biomass of the first and last day of summer. The MEPPS draws hourly temperature and solar radiation from MCIP for use in the biogenic processor. Land cover and vegetation are provided in gridded ARC/INFO coverage. The biogenic modeling input data are then provided to BEIS-2 and output as hourly gridded emission values of the VOCs isoprene, monoterpene, and “other” (unspecified); along with NO to the EMPRO speciation processor, where they are grouped with chemical species from other source types depending upon the conventions of either the CB4 or RADM2 speciation split factors (Section 4.2.5).

4.2.4.2 Mobile Source Emissions

Emissions from mobile sources to the air are established as one of the primary contributors to pollution problems in many localities. Unlike many anthropogenic emissions, mobile source emissions are strongly affected by the rapid variations of atmospheric temperature and anthropogenically-influenced, geographically-varying factors. Consequently, it is necessary to model hourly mobile emissions, rather than to temporally disaggregate annual totals. The capability to do this is in the MEPPS mobile-source emission processor. For gaseous emissions the mobile source processor estimates hourly emissions of VOC total organic gases (TOG), carbon monoxide (CO), and oxides of nitrogen (NOx) from on-road mobile sources (vehicles). The processor, which is located in the EMPRO module of MEPPS, uses a combination of air temperature data at 1.5 m above the surface (provided by MM5 through MCIP), mobile source emission factors (computed by the EPA regulatory model Mobile 5a for gaseous emissions from

on-road mobile sources), fleet vehicle type composition, road type, and traffic data in the form of vehicle miles traveled (VMT) to generate emission estimates. Vehicle emission controls, and Inspection and Maintenance programs may be accounted for in the user-defined input settings for Mobile 5a (U.S. EPA, 1991; U.S. EPA, 1996). The VMT data are usually available by county, or occasionally by specific road segments. The resulting county or road segment-specific hourly emissions are spatially allocated to the cells of a user-defined study grid. The gridded emission data are combined with corresponding species output from the mobile source particulate emission model, and allocated to different groups of lumped species for processing by the Speciation Processor (Section 4.2.5).

Emissions of particulate species (particulate matter less that 10 micrometer and 2.5 micrometers in diameter - PM_{10} and $PM_{2.5}$, respectively) from mobile sources are modeled analogously to gaseous emissions, using vehicle fleet composition, road type (urban or rural), and VMT data. The mobile particulate emission factors are modeled with PART5 (U.S. EPA, 1995), the particulate companion of Mobile 5a. Vehicle emission controls, Inspection and Maintenance programs, and use of reformulated fuel may be accounted for with the input settings of PART5. In addition input information for road silt content and precipitation is required. The particulate species modeled include lead, direct and indirect particulate sulfate (any remaining sulfur in fuel is assumed to be exhausted as gaseous SO_2), total exhaust particulate (sum of lead, direct sulfate, and carbon including soluble organic material and other remaining carbon), and (separately) soluble organic fraction (SOF) and a remainder carbon portion (RCP), which are added to the mobile source emission output file.

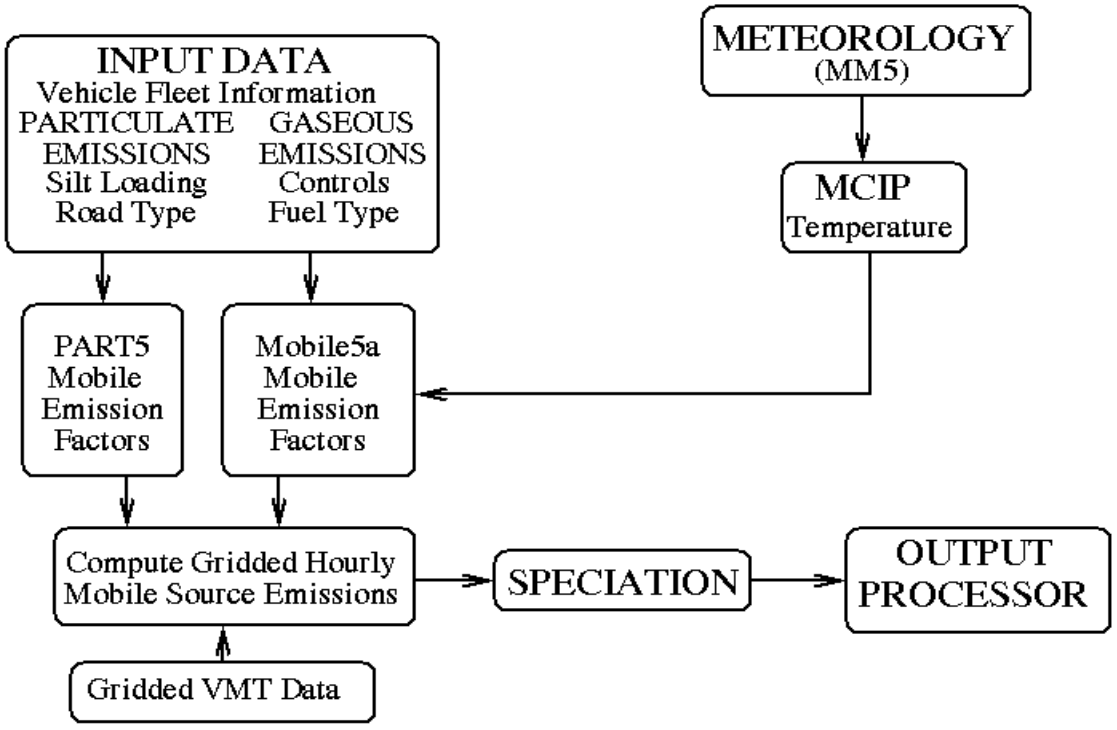


Figure 4-5 General Flow of Mobile Source Emission Modeling

The procedure by which mobile source emission data are estimated in MEPPS and flow diagrams for the process are given in Section 6.5.3.4 of the *Models-3 Volume 9B: User Manual*. Briefly, the sequence is as follows:

- VMT vehicle fleet data files are established for the study area (gridded spatial domain) of interest by either extracting county-level annual aggregate VMT data from the annual emission input files previously established by INPRO, or by loading "link-node" VMT data that are available for specific road segments (links) between nodes with geographic coordinates . The link-node data are generally available only for selected urban areas and dates in conjunction with special studies. The process is similar for VMT data which are occasionally available by quarter section (1/4 square mile) areas.

- ARC/INFO® spatial coverage files of surrogate data (Federal Highway Administration major highways, or United States Census Tiger Line road coverages are provided) are used to spatially allocate county-level aggregate VMT data to the cells of the gridded domain being used with a particular study. County area may also be used as a coarse surrogate coverage.

- Spatial allocation ratios are computed for use in assigning county-level VMT data to the surrogate coverages. The EMPRO calculates the proportion of road links or county area in the spatial domain attributable to each grid cell overlain by the road link (FHA or TIGER/LINE) or county.

- Mobile source emission factors are computed using Mobile 5a and/or PART 5- U.S. EPA regulatory models. Mobile 5a requires user-defined information on driving operations, vehicle fleet and fuel use, and hourly ambient temperature data. PART 5 requires user-defined information on vehicle fleet and fuel use, emission controls, non-attainment, road dust silt content, moisture, and percent of unpaved roads by geographic area (usually county). Temperature and moisture data are from the MM5 model as processed by MCIP.

- Hourly mobile emissions are computed for each grid cell, with adjustments applied to VMT to indirectly reflect the effect of temperature on gaseous emissions, and moisture on re-entrained dust for particulate emissions.

- For mobile emissions of VOC, hourly gridded mobile emissions are speciated using either RADM 2.0 or CB-4 emission profile splits. Speciation is not needed for particulate emission data.

- The hourly, gridded, speciated mobile emission data are merged with gridded, speciated hourly area-source emission data in OUTPRO, and converted to NetCDF I/O API format,

to provide a two dimensional emission data set acceptable to the chemical-transport model and other Models-3 framework applications.

The Mobile 5a Model

Detailed descriptions of Mobile 5a are available from EPA publications (US EPA 1991, US EPA 1996). An optional Mobile 5b has also been adopted (US EPA 1996) to accommodate slight modifications in Inspection and Modification credits for hybrid fuels. Both Mobile 5a and 5b are improvements in the Mobile 4.1 model (US EPA, July 1991). Mobile 6 is in development and is tentatively expected in late 1999. A new off-road mobile emission model is also due in late 1998. Portions of the following description of Mobile are adapted from Wilkinson et al (1994). The incorporation of Mobile 5a into MEPPS was extensively revised from its treatment in GEMAP, including:

- The application of Mobile 5a factors was revised to substantially reduce redundancy and computational space required. The application of Mobile 5a in GEMAP computed specific emission factors for individual state/counties by area type/road type and hour. The combinations of hour and road type were derived by mapping operating modes (percent of hot and cold starts) to the hours and road types that used them, causing a duplication of Mobile 5a runs and factors. It was necessary to recompute factors if there was a change in how the emission factors were used by hours or road type. The computed mobile emission factors were merged into permanent (for the processing run) emission factor tables without regard to calendar year. In MEPPS, Mobile 5a emission factors are computed and stored by calendar year, state/county, and operating mode. Also, the system now has separate user-specified tables that allocate emission factors by hour and road type, using operating mode. The tables are used directly in the emission estimate calculation. In addition start and end times may now be specified for mobile emission runs rather than number of complete hours. This has also shortened the processing time for county-level mobile emission processing.

- Calculations were separated into county-level, link-node level, and land-survey level options, depending upon the spatial detail of VMT information available to the user.

- The ability to assign alias identification by state or county was added. This allows the user to assign the values in a Mobile input file for a given area to a similar area which lacks specific input data.

- Geographic coverages of major highways (from the Federal Highway Administration) and all roads (TIGER-Line data) were made available as surrogate data to allow better spatial allocation of mobile emissions.

- Mobile emission data are now subject to the additional quality control and ARC-INFO® based visualization capabilities in MEPPS.

Mobile 5a is an ANSI FORTRAN 77 computer program designed to estimate hydrocarbon (HC), carbon monoxide (CO), and oxides of nitrogen (NO_X) emission factors for gasoline-fueled and diesel-fueled highway motor vehicles. The computation methods that are embedded in Mobile 5a are based on the procedures that are presented in the *Compilation of Air Pollutant Emission Factors -- Volume XX: Highway Mobile Sources* (US EPA, 1995). Mobile 5a computes emissions factors for eight vehicle categories in two regions of the country (high-altitude and low-altitude). The eight vehicle categories include the following:

- LDGV – light-duty gasoline vehicles;
- LDGT1 -- light-duty gasoline trucks (up to 6000 pounds);
- LDGT2 -- light-duty gasoline trucks (6001 to 8500 pounds);
- HDGV – heavy-duty gasoline vehicles (over 8500 pounds);
- LDDV – light-duty diesel vehicles;
- LDDT – light-duty diesel trucks (0 to 8500 pounds);
- HDDV – heavy-duty diesel vehicles (over 8500 pounds); and
- MC -- motorcycles.

The Mobile 5a emission factors depend on various conditions including, but not limited to, ambient temperature, vehicle speed, operating modes, and vehicle mileage accrual rates. Much of the data required by Mobile 5a may be specified by the user through the Mobile input file. Mobile computes emissions factors for any year from 1960 to 2020. This date range is important for mobile-source emission estimated projections, and for the application of regulatory control factors. Mobile version 5a.01 (which was modified for use in GEMAP/EMS-95 and later for MEPPS) is currently implemented in the EMPRO module of MEPPS. Consult the *User's Guide to MOBILE 5, EPA-AA-TEB-92-01* for further details on Mobile 5a. Mobile model documentation may be obtained from the EPA Office of Mobile Sources World Wide Web home page located at: **http://www.epa.gov/OMSWWW/models.htm**.

A comprehensive discussion of the technical formulation of Mobile 5a is found in the above references. This section contains a description of modifications to Mobile 5a for use in GEMAP and later in MEPPS. Mobile 5a was modified for use in EMS-95 to compute and report diurnal evaporative emissions factors (grams/mile) separately. The unmodified Mobile 5a model computes and reports diurnal evaporative emission factors as part of a composite evaporative emission factor. Also, Mobile 5a was modified to report a total non-diurnal evaporative emission factor. The total non-diurnal evaporative emission factor includes hot soak, crankcase blow-by, running losses, and resting losses. In the MEPPS EMPRO module, the Mobile SAS® table generators have been rewritten and segmented for greater computational efficiency, as have been the VMT and surrogate coverage grid processors and mobile source emission calculation procedures. The technical procedure and rationale are the same, but processing time is shortened by at least a factor of two for regional modeling of spatial domains.

The mobile-source emission processor relies on a SAS® lookup table to find appropriate emissions factors to compute the motor vehicle emission estimates. The SAS® lookup table is generated through iterative runs of Mobile 5a. The necessary number of runs of Mobile 5a is performed automatically, and is based on the standard Mobile ASCII input file supplied by the user. For urban scale modeling, an input file for one state may suffice. However, for regional modeling, multiple Mobile 5a ASCII input files can be concatenated to one file and run through the processor. This capability is necessary to handle study domains where motor vehicle activity differs spatially and temporally. For example, in a multiple-state study domain, it is unlikely that adjoining states have the same inspection and maintenance (I/M) program or the same vehicle fleet distribution (to name just two inputs to Mobile 5a). Differences in regional inputs to Mobile 5a such as I/M programs and vehicle fleet distributions result in different motor vehicle emissions factors. A concatenated input file template (based on example values used for the OTAG project) is provided which may be copied and edited. In MEPPS, the Mobile input file (*m5a.mv*) is located in the directory structure at:

$EMS_HOME*/project/*$EMS_PROJECT/raw_data/*$EMS_DOMAIN*/common/.

The only difference in the concatenated input file from the original input file is that the state title lines contain state (and where needed, county) FIPS identifier codes to identify the area for which each section of the Mobile 5a input file is applicable:

- FIPS state code -- Mobile input file applies to a state; or
- FIPS state code and FIPS county code -- Mobile input file applies to a particular county.

The mobile-source emission processor varies the vehicle speed and ambient temperature records of the user-supplied input file and runs Mobile for each variation. The Mobile source processor varies the vehicle speeds from 4 miles per hour to 64 miles per hour in increments of 2 miles per hour, although the user may adjust the increment (Mobile supports computation of emission factors for speeds between 2.5 MPH and 65 MPH). The mobile-source processor varies the minimum ambient temperature from 50° F to 110° F in increments of 2° F, and the mobile source processor varies the maximum ambient temperature from 50° F to 110° F in increments of 2° F (Mobile 5a supports computation of exhaust emissions factors for temperatures between 0° F and 110° F and evaporative emissions factors for temperatures between 40° F and 110° F). The vehicle speed and ambient temperature values can be set interactively in EMPRO under the mobile source model, using the "Generate Mobile Emission Factors" screen.

In MEPPS, the mobile-source processor generates two emission factor SAS® lookup tables. These are compact tables that contain the information held in seven generated SAS lookup tables in EMS-95. They are:

- State/area type/facility type diurnal emissions factors (I/M and non-I/M HC diurnal evaporative emissions factors for eight vehicle categories by state, minimum ambient temperature, maximum ambient temperature, and calendar year). The user specifies

whether the operating mode varies by the hour of the day in the Temporal Allocation screen of the mobile emission model of EMPRO);

- State/area-type/facility-type non-diurnal emissions factors (I/M and non-I/M HC [evaporative and exhaust], CO [exhaust only], and NO_X [exhaust only] emissions factors for eight vehicle categories by state, area type [urban or rural], facility type [eg. interstate, collector, arterial, local], vehicle speed, ambient temperature, and calendar year. The user can interactively specify whether the operating mode varies by hour of the day when establishing temporal profiles in the Temporal Allocation screen of the mobile emission model of EMPRO.

Operating mode is an important variable in the computation of motor vehicle emissions factors. Attention is specifically called to operating mode because the mobile source processor uses up to four different operating mode mixes to compute emissions factors for the Mobile 5a lookup tables (refer to the Mobile 5a user's guide for further discussion of operating modes).

If area type/facility type records are to be used in the Mobile-generated lookup tables, the user must specify the mix of operating modes. The following example of operating mode mixes was used for the Lake Michigan Ozone Study: 5% PCCN, 12.1% PCHC, and 10.9% PCCC, where PCCN is percent VMT generated by non-catalyst vehicles in cold-start mode, PCHC is percent VMT generated by catalyst vehicles in hot-start mode, and PCCC is percent VMT generated by catalyst vehicles in cold-start mode. If hourly records are used in the Mobile-generated lookup tables, the user must define the operating mode mixes by time of day, consistent with Mobile 5a guidance. The following is an example of the use of four operating mode mixes:

- 0000 to 0700 operating mode is 12.9% PCCN, 7% PCHC, and 17% PCCC;
- 0700 to 0900 operating mode is 15% PCCN, 10% PCHC, and 15.4% PCCC;
- 0900 to 1600 operating mode is 5% PCCN, 12.1% PCHC, and 10.9% PCCC;
- 1600 to 1800 operating mode is 10.1% PCCN, 9.1% PCHC, and 13.9% PCCC;
- 1800 to 2200 operating mode is 5% PCCN, 12.1% PCHC, and 10.9% PCCC;
- 2200 to 0000 operating mode is 12.9% PCCN, 7% PCHC, and 17% PCCC.

As with the vehicle speeds and ambient temperatures, the operating mode mixes can be changed interactively on the Operating mode screen in THE MEPPS EMPRO module under Models, Mobile, Mobile Source.

The mobile source processor generates emission factors for the following area type (urban or rural) and facility type (interstate, local, etc.) combinations:

- rural/principal arterial - interstate
- urban/principal arterial - interstate
- rural/principal arterial - other
- urban/principal arterial - free/express-ways

- rural/minor arterial
- urban/principal arterial - other
- rural/major collector
- urban/collector
- rural/minor collector
- urban/minor arterial
- rural/local
- urban/local

As with vehicle speeds, ambient temperatures, and operating modes; area type/facility type combinations can be changed interactively using the “Generate Mobile Emission Factors" screen under EMPRO, Models, Mobile, Mobile Source to edit the ASCII input file . When changes are made, the same changes are automatically made to the SAS® data sets.

User Input Data

The mobile source emission processor requires user-defined specifications using interactive screens and an input file. While some of the specifications are required, some are not required. In each case, there is provision to import the data file through IDA or in the mobile source processor of MEPPS.

The principal input data ASCII files to the mobile source model include the following (environment variables are defined in Chapter 6 of the *Models 3 Volume 9B: User Manual*):

- On-network link-specific area type/facility type (*$EMS/onnet.mv)*
- On-network link-specific percentage of vehicles that fall under an I/M program *($EMS/onnetim.mv)*
- On-network link-specific daily or hourly VMT *($EMS/onnetvmt.mv*);
- Hourly or daily, link-specific or area type/facility type-specific vehicle mix
- Off-network, area type/ facility type average speed *($EMS_LOC/offnetspd.mv)*
- Off-network, area type/facility type VMT *($EMS/offnvmt.mv)*;
- Off-network, area type/facility type-specific vehicle mix profile *($EMS_LOC/offvmix.mv)*
- Public land survey quarter sections area type/ facility type hourly or daily VMT, hourly speeds, and daily vehicle mix profile *($EMS/ofnvmtp.mv)*;
- Area type/facility type seasonal and daily adjustment factors *($EMS/adjstvmt.mv)*
- Area type/facility type hourly average speed profile *($EMS_CAT/spdadju.mv)*
- On-network, link-specific hourly or daily average speed *($EMS_GRD/onnetspd.mv)*
- Area type/facility type hourly VMT fractional profile *($EMS/fracvmtu.mv)*

If off-network VMT is to be used to compute emissions estimates (typical when county VMT data are taken from regional emission inventories), the mobile emission processor can assign VMT to grid cells using ARC/INFO® coverage files for either county area, Federal Highway Administration (FHA) major highways, or TIGER/LINE road data. These coverages for the

contiguous United States are provided with MEPPS. Subsets of the coverages for the spatial domain of interest are extracted either when a grid is established or during mobile source processing.

If Public Land Survey Quarter Section-based VMT is to be used to compute emissions estimates, the mobile source emission processor requires an ARC/Info® export data set of the polygon-network system.

Gridding VMT

After the ASCII user input (foundation) data files have been read and checked, the user directs the mobile source emission processor to prepare the necessary network coverages (unless they were prepared when the grid was established). The on-network system is prepared from the user-provided ASCII input files. The off-network system is prepared via county boundary, FHA, or TIGER/LINE data file extracts. The polygon system is prepared from an ARC/INFO® export coverage. The networks are gridded by overlaying the emission modeling grid on the network coverages in much the same manner that the area source spatial surrogates are gridded. Each link in the networks (or area type/facility type polygon) are length (or area) apportioned to a grid cell in the emissions modeling domain. Once the networks have been gridded, the corresponding VMT can also be gridded. Equations 4-25 through 4-30 show how the on-network, off-network, and polygon VMT are gridded respectively.

$$lenratio_{i,j,k,l,m} = lengrid_{i,j,k,l,m} / lenpar_{i,j,k} \quad (4\text{-}25)$$

$$VMT_{i,j,k,l,m} = vmtorig_{i,j,k} * lenratio_{i,j,k,l,m} \quad (4\text{-}26)$$

$$cellpct_{i,j,a,f,l,m} = cellsum_{i,j,a,f,l,m} / ctysum_{i,j,a,f} \quad (4\text{-}27)$$

$$VMT_{i,j,a,f,l,m} = vmtorig_{i,j,a,f} * cellpct_{i,j,a,f,l,m} \quad (4\text{-}28)$$

$$areapct_{i,j,p,a,f,l,m} = areagrd_{i,j,p,a,f,l,m} / areapar_{i,j,p} \quad (4\text{-}29)$$

$$VMT_{i,j,p,a,f,l,m} = vmtorig_{i,j,p,a,f} * areapct_{i,j,p,a,f,l,m} \quad (4\text{-}30)$$

where lenratio is the percentage of a link in a given grid cell
lengrid is the length of a link in a given grid cell
lenpar is the total length of the link
VMT is the gridded VMT value
vmtorig is the original VMT
cellpct is the percent of the FHA or TIGER/Line-based area type/facility type roadway in a given cell
cellsum is the total length of FHA or TIGER/Line-based area type/facility type roadway in a given cell
ctysum is the total length of the FHA or TIGER/Line-based area type/facility type roadway in a county
areapct is the percent of the polygon-based area type/facility type roadway in a given cell

areagrd is the total length of the polygon-based area type/facility type roadway in a given cell
areapar is the total length of the polygon-based area type/facility type roadway in a county
i is the state index
j is the county index
k is the link index for on-network systems
l is the east-west grid cell index
m is the north-south grid cell index
a is the area type index for off-network systems
f is the facility type index for off-network systems
p is the polygon index for Public Land Survey Quarter Sections network systems.

For on-network and polygon VMT, the indices may also include an identifier for hour since polygon and on-network VMT can also be supplied on an hourly basis.

Apply Default Information

If the user supplies limited data to the mobile-source emission processor, it can apply a variety of default values to compute motor vehicle emissions estimates. These defaults include vehicle mix, speeds, VMT fractional profiles, and I/M vehicle percentages. If the user supplies limited data, the mobile-source emission processor applies the following defaults:

Default Vehicle Mix Profile

Vehicle Class	Percentage
LDGV	0.618
LDGT1	0.177
LDGT2	0.077
HDGV	0.035
LDDV	0.008
LDDT	0.002
HDDV	0.077
MC	0.008

Default Speed Profile

Area Type	Facility Type	Speed
0	1	60
0	4	56
0	6	56
0	7	54
0	8	40
0	9	35
1	1	60
1	2	59
1	4	55
1	5	30
1	6	55
1	9	30

Default Hourly VMT Fractional Profile

Emission	Hour	1	2	3	4	5	6	7	8	9	10	11	12
Diurnal		0.000	0.000	0.000	0.000	0.000	0.129	0.021	0.100	0.095	0.095	0.166	0.199
Other		0.016	0.010	0.003	0.006	0.010	0.026	0.053	0.064	0.055	0.048	0.050	0.052

	13	14	15	16	17	18	19	20	21	22	23	24
Diurnal	0.079	0.116	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
Other	0.054	0.055	0.059	0.070	0.074	0.070	0.058	0.046	0.037	0.033	0.028	0.022

If the user does not specify what the percentage of vehicles are under an I/M program, the mobile source emission processor assumes that no vehicles are under an I/M program. The result is higher emission estimates.

The mobile source emission processor does not override user-supplied data. Default information are applied only when data are missing from the ASCII user input files.

Add Temperatures and Adjust VMT

Prior to computing the motor vehicle emission estimates, the mobile-source emission processor adds the gridded, hourly temperatures and adjusts the VMT to the specific modeling day. The temperature data are used to obtain the correct emission factor from the Mobile emission factors lookup tables. Through the application of Equations 4-31 through 4-34, the day-specific, diurnal and nondiurnal (other than full days), hourly VMT are computed, respectively.

$$dvmt_{i,j,l,h,m,n} = ddayvmt_{i,j,l,m,n} * adjday * adjmonth * dvmt\_prof_{i,j,l,h} \quad (4\text{-}31)$$

$$ovmt_{i,j,l,h,m,n} = odayvmt_{i,j,l,m,n} * adjday * adjmonth * ovmt\_prof_{i,j,l,h} \quad (4\text{-}32)$$

$$dvmt_{i,j,a,f,h,m,n} = ddayvmt_{i,j,a,f,m,n} * adjday * adjmonth * dvmt\_prof_{i,j,a,f,h} \quad (4\text{-}33)$$

$$ovmt_{i,j,a,f,h,m,n} = odayvmt_{i,j,a,f,m,n} * adjday * adjmonth * ovmt\_prof_{i,j,a,f,h} \quad (4\text{-}34)$$

where

dvmt is the diurnal VMT;
dayvmt is the total day diurnal VMT;
adjday is the day-specific VMT adjustment factor supplied through an ASCII input file;
adjmonth is the month-specific VMT adjustment factor supplied through an ASCII input file;
dvmt_prof is the hour-specific, diurnal VMT fractional profile factor;
ovmt is the nondiurnal VMT;
odayvmt is the total day nondiurnal VMT;
ovmt_prof is the hour-specific, nondiurnal VMT fractional profile factor;
i is the state index;
j is the county index;
h is the hour index;
l is the link identifier index;
a is the area type index;
f is the facility type index;
m is the east-west grid cell index; and
n is the north-south grid cell index.